PROPYL DODECANOATE

Other names: Propyl laurate
Inchi: InChI=1S/C15H30O2/c1-3-5-6-7-8-9-10-11-12-13-15(16)17-14-4-2/h3-14H2,1-2H3
InchiKey: FTBUKOLPOATXGV-UHFFFAOYSA-N
Formula: C15H30O2
SMILES: CCCCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 242.40
CAS: 3681-78-5

Physical Properties

Property code	Value	Unit	Source
af	0.7973		Cheméo Relay (1.0)
hf	-673.26	kJ/mol	Cheméo Relay (1.0)
hfus	37.39	kJ/mol	Joback Method
hvap	84.70	kJ/mol	NIST Webbook
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-5.19		Cheméo Relay (1.0)
logp	4.861		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1691.30		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1691.30		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1694.00		NIST Webbook
ripol	1897.00		NIST Webbook
ripol	1927.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1897.00		NIST Webbook
tb	550.83	K	Cheméo Relay (1.0)
tc	725.06	K	Cheméo Relay (1.0)
tf	265.88	K	Cheméo Relay (1.0)
vc	0.898	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.70	J/mol×K	758.49	Joback Method
cpg	714.65	J/mol×K	786.41	Joback Method
cpg	638.14	J/mol×K	646.81	Joback Method
cpg	654.83	J/mol×K	674.73	Joback Method
cpg	670.81	J/mol×K	702.65	Joback Method
cpg	686.10	J/mol×K	730.57	Joback Method
cpg	620.74	J/mol×K	618.89	Joback Method
dvisc	0.0006264	Pa×s	426.94	Joback Method
dvisc	0.0011647	Pa×s	378.96	Joback Method
dvisc	0.0025922	Pa×s	330.97	Joback Method
dvisc	0.0003819	Pa×s	474.93	Joback Method
dvisc	0.0002549	Pa×s	522.92	Joback Method
dvisc	0.0001822	Pa×s	570.90	Joback Method
dvisc	0.0001371	Pa×s	618.89	Joback Method
hvapt	66.90	kJ/mol	437.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56938e+01
Coeff. B	-5.10061e+03
Coeff. C	-9.78450e+01
Temperature range (K), min.	428.92
Temperature range (K), max.	589.12

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3681785&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume