Dodecyl propionate

Other names: Dodecyl propionate
propionic acid, dodecyl ester
Inchi: InChI=1S/C15H30O2/c1-3-5-6-7-8-9-10-11-12-13-14-17-15(16)4-2/h3-14H2,1-2H3
InchiKey: FVGJPCFYGPKBKJ-UHFFFAOYSA-N
Formula: C15H30O2
SMILES: CCCCCCCCCCCCOC(=O)CC
Mol. weight [g/mol]: 242.40

Physical Properties

Property code	Value	Unit	Source
af	0.7954		Cheméo Relay (1.0)
gf	-158.50	kJ/mol	Joback Method
hf	-669.46	kJ/mol	Cheméo Relay (1.0)
hfus	37.39	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Cheméo Relay (1.0)
ie	9.64	eV	Cheméo Relay (1.0)
log10ws	-5.15		Cheméo Relay (1.0)
logp	4.861		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1672.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1959.00		NIST Webbook

ripol	1911.00		NIST Webbook
ripol	1979.00		NIST Webbook
ripol	1960.00		NIST Webbook
tb	548.29	K	Cheméo Relay (1.0)
tc	725.60	K	Cheméo Relay (1.0)
tf	271.63	K	Cheméo Relay (1.0)
vc	0.900	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6221938&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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