2-Propenoic acid, 2-methyl-, decyl ester

Other names: Decyl methacrylate
Methacrylic acid, decyl ester
n-Decyl methacrylate
Inchi: InChI=1S/C14H26O2/c1-4-5-6-7-8-9-10-11-12-16-14(15)13(2)3/h2,4-12H2,1,3H3
InchiKey: GTBGXKPAKVYEKJ-UHFFFAOYSA-N
Formula: C14H26O2
SMILES: C=C(C)C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 226.35
CAS: 3179-47-3

Physical Properties

Property code	Value	Unit	Source
gf	-87.63	kJ/mol	Joback Method
hf	-461.45	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.246		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	1556.00		NIST Webbook
rinpol	1557.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1841.00		NIST Webbook
tb	592.57	K	Joback Method
tc	765.39	K	Joback Method
tf	250.70	K	NIST Webbook
tf	250.70	K	NIST Webbook
tf	250.70 ± 0.10	K	NIST Webbook
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	621.51	J/mol×K	736.59	Joback Method
cpg	545.45	J/mol×K	592.57	Joback Method
cpg	562.05	J/mol×K	621.37	Joback Method
cpg	577.93	J/mol×K	650.18	Joback Method
cpg	593.13	J/mol×K	678.98	Joback Method
cpg	607.65	J/mol×K	707.78	Joback Method
cpg	634.72	J/mol×K	765.39	Joback Method
cpl	452.90	J/mol×K	298.15	NIST Webbook
cpl	452.50	J/mol×K	298.15	NIST Webbook
hfust	30.55	kJ/mol	250.70	NIST Webbook
hfust	30.55	kJ/mol	250.70	NIST Webbook
hfust	30.55	kJ/mol	250.70	NIST Webbook
hvapt	62.70	kJ/mol	445.50	NIST Webbook
sfust	121.90	J/mol×K	250.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28805e+01
Coeff. B	-3.86144e+03
Coeff. C	-8.37640e+01
Temperature range (K), min.	390.40
Temperature range (K), max.	593.93

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3179473&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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