Z-8-METHYL-9-TETRADECENOIC ACID

Inchi: InChI=1S/C15H28O2/c1-3-4-5-8-11-14(2)12-9-6-7-10-13-15(16)17/h8,11,14H,3-7,9-10,1
InchiKey: QCLNEWABNXOXBO-FLIBITNWSA-N
Formula: C15H28O2
SMILES: CCCC/C=C\C(C)CCCCCCC(=O)O
Mol. weight [g/mol]: 240.39

Physical Properties

Property code	Value	Unit	Source
gf	-112.54	kJ/mol	Joback Method
hf	-624.02	kJ/mol	Cheméo Relay (1.0)
hfus	36.97	kJ/mol	Joback Method
hvap	106.36	kJ/mol	Cheméo Relay (1.0)
ie	9.05	eV	Cheméo Relay (1.0)
log10ws	-4.43		Cheméo Relay (1.0)
logp	4.794		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
tb	572.99	K	Cheméo Relay (1.0)
tc	762.03	K	Cheméo Relay (1.0)
tf	279.63	K	Cheméo Relay (1.0)
vc	0.812	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.68	J/mol×K	692.37	Joback Method
cpg	656.79	J/mol×K	721.23	Joback Method
cpg	671.19	J/mol×K	750.09	Joback Method
cpg	684.92	J/mol×K	778.95	Joback Method
cpg	697.99	J/mol×K	807.81	Joback Method
cpg	710.45	J/mol×K	836.67	Joback Method
cpg	722.33	J/mol×K	865.54	Joback Method
dvisc	0.0063588	Pa×s	349.48	Joback Method
dvisc	0.0014345	Pa×s	406.63	Joback Method

dvisc	0.0004671	Pa×s	463.78	Joback Method
dvisc	0.0001945	Pa×s	520.92	Joback Method
dvisc	0.0000963	Pa×s	578.07	Joback Method
dvisc	0.0000541	Pa×s	635.22	Joback Method
dvisc	0.0000335	Pa×s	692.37	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=U130845&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume