

9-Octadecenoic acid, tetrahydrofurfuryl ester

Inchi:	InChI=1S/C23H42O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-23(24)26-21-22-18-17
InchiKey:	GIPDEPRRXIBGNF-MDZDMXLPSA-N
Formula:	C23H42O3
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	366.58

Physical Properties

Property code	Value	Unit	Source
gf	-60.49	kJ/mol	Joback Method
hf	-717.15	kJ/mol	Joback Method
hfus	60.23	kJ/mol	Joback Method
hvap	80.67	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.746		Crippen Method
mcvol	333.080	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
tb	848.32	K	Joback Method
tc	1042.07	K	Joback Method
tf	453.52	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.17	J/molxK	848.32	Joback Method
cpg	1190.39	J/molxK	1009.78	Joback Method
cpg	1174.48	J/molxK	977.49	Joback Method
cpg	1157.55	J/molxK	945.20	Joback Method
cpg	1139.56	J/molxK	912.90	Joback Method
cpg	1120.45	J/molxK	880.61	Joback Method
cpg	1205.36	J/molxK	1042.07	Joback Method
dvisc	0.0000538	Paxs	848.32	Joback Method
dvisc	0.0000721	Paxs	782.52	Joback Method
dvisc	0.0001020	Paxs	716.72	Joback Method

dvisc	0.0001549	Paxs	650.92	Joback Method
dvisc	0.0002582	Paxs	585.12	Joback Method
dvisc	0.0004900	Paxs	519.32	Joback Method
dvisc	0.0011199	Paxs	453.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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

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