2-Hexadecylidene-1,3-dithiolane

Inchi: InChI=1S/C19H36S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-20-17-18-21-19/h16H
InchiKey: DTKFBFMAVWGTAQ-UHFFFAOYSA-N
Formula: C19H36S2
SMILES: CCCCCCCCCCCCCCCC=C1SCCS1
Mol. weight [g/mol]: 328.62

Physical Properties

Property code	Value	Unit	Source
gf	278.54	kJ/mol	Joback Method
hf	-188.12	kJ/mol	Joback Method
hfus	45.47	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.789		Crippen Method
mcvol	296.110	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	756.37	K	Joback Method
tc	953.26	K	Joback Method
tf	496.29	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.54	J/mol×K	756.37	Joback Method
cpg	889.41	J/mol×K	789.18	Joback Method
cpg	908.24	J/mol×K	822.00	Joback Method
cpg	926.08	J/mol×K	854.81	Joback Method
cpg	943.00	J/mol×K	887.63	Joback Method
cpg	959.07	J/mol×K	920.44	Joback Method
cpg	974.35	J/mol×K	953.26	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R391114&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume