2-Heptadecylidene-1,3-dithiolane

Inchi: InChI=1S/C20H38S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-21-18-19-22-20/h1
InchiKey: GWQMQVPESVIDPM-UHFFFAOYSA-N
Formula: C20H38S2
SMILES: CCCCCCCCCCCCCCCCC=C1SCCS1
Mol. weight [g/mol]: 342.65

Physical Properties

Property code	Value	Unit	Source
gf	286.96	kJ/mol	Joback Method
hf	-208.76	kJ/mol	Joback Method
hfus	48.06	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.179		Crippen Method
mcvol	310.200	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2687.00		NIST Webbook
rinpol	2687.00		NIST Webbook
tb	779.25	K	Joback Method
tc	975.43	K	Joback Method
tf	507.56	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.23	J/mol×K	779.25	Joback Method
cpg	949.31	J/mol×K	811.95	Joback Method
cpg	968.34	J/mol×K	844.64	Joback Method
cpg	986.39	J/mol×K	877.34	Joback Method
cpg	1003.52	J/mol×K	910.04	Joback Method
cpg	1019.81	J/mol×K	942.73	Joback Method
cpg	1035.30	J/mol×K	975.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R391109&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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