2-Pentadecylidene-1,3-dithiolane

Inchi: InChI=1S/C18H34S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-19-16-17-20-18/h15H,2-1
InchiKey: YQWGGBRVNHWRES-UHFFFAOYSA-N
Formula: C18H34S2
SMILES: CCCCCCCCCCCCCCC=C1SCCS1
Mol. weight [g/mol]: 314.59

Physical Properties

Property code	Value	Unit	Source
gf	270.12	kJ/mol	Joback Method
hf	-167.48	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	68.64	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	7.399		Crippen Method
mcvol	282.020	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	2469.00		NIST Webbook
tb	733.49	K	Joback Method
tc	931.62	K	Joback Method
tf	485.02	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.84	J/mol×K	733.49	Joback Method
cpg	830.49	J/mol×K	766.51	Joback Method
cpg	849.11	J/mol×K	799.53	Joback Method
cpg	866.74	J/mol×K	832.56	Joback Method
cpg	883.45	J/mol×K	865.58	Joback Method
cpg	899.30	J/mol×K	898.60	Joback Method
cpg	914.36	J/mol×K	931.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R391154&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