3-Sulfanylhexyl Octadodecanoate

Inchi: InChI=1S/C24H48O2S/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-24(25)26-22-21-2
InchiKey: KYFUWFDMLLFQOE-UHFFFAOYSA-N
Formula: C24H48O2S
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCCC(S)CCC
Mol. weight [g/mol]: 400.70

Physical Properties

Property code	Value	Unit	Source
gf	-55.77	kJ/mol	Joback Method
hf	-750.29	kJ/mol	Joback Method
hfus	61.22	kJ/mol	Joback Method
hvap	84.52	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	8.280		Crippen Method
mcvol	372.810	ml/mol	McGowan Method
pc	863.02	kPa	Joback Method
rinpol	2816.00		NIST Webbook
tb	887.23	K	Joback Method
tc	1086.22	K	Joback Method
tf	453.86	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.53	J/mol×K	887.23	Joback Method
cpg	1246.28	J/mol×K	920.40	Joback Method
cpg	1265.75	J/mol×K	953.56	Joback Method
cpg	1283.98	J/mol×K	986.73	Joback Method
cpg	1301.02	J/mol×K	1019.89	Joback Method
cpg	1316.93	J/mol×K	1053.06	Joback Method
cpg	1331.75	J/mol×K	1086.22	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=R519674&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