3-Sulfanylhexyl Tetradodecanoate

Inchi: InChI=1S/C20H40O2S/c1-3-5-6-7-8-9-10-11-12-13-14-16-20(21)22-18-17-19(23)15-4-2/h
InchiKey: LMBOHFYTEYIWQI-UHFFFAOYSA-N
Formula: C20H40O2S
SMILES: CCCCCCCCCCCCCC(=O)OCCC(S)CCC
Mol. weight [g/mol]: 344.60

Physical Properties

Property code	Value	Unit	Source
gf	-89.45	kJ/mol	Joback Method
hf	-667.73	kJ/mol	Joback Method
hfus	50.86	kJ/mol	Joback Method
hvap	75.62	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.719		Crippen Method
mcvol	316.450	ml/mol	McGowan Method
pc	1096.44	kPa	Joback Method
rinpol	2412.00		NIST Webbook
tb	795.71	K	Joback Method
tc	981.41	K	Joback Method
tf	408.78	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.31	J/mol×K	795.71	Joback Method
cpg	995.50	J/mol×K	826.66	Joback Method
cpg	1013.64	J/mol×K	857.61	Joback Method
cpg	1030.78	J/mol×K	888.56	Joback Method
cpg	1046.94	J/mol×K	919.51	Joback Method
cpg	1062.14	J/mol×K	950.46	Joback Method
cpg	1076.43	J/mol×K	981.41	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519689&Units=SI

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