Acetic acid, 2,2'-thiobis-, dibutyl ester

Other names: Thiodiglycollic acid dibutyl ester
dibutyl 2,2'-thiobisacetate
Thiodiglycolic acid, diethyl ester
Inchi: InChI=1S/C12H22O4S/c1-3-5-7-15-11(13)9-17-10-12(14)16-8-6-4-2/h3-10H2,1-2H3
InchiKey: RIQXZINBEMXOOE-UHFFFAOYSA-N
Formula: C12H22O4S
SMILES: CCCCOC(=O)CSCC(=O)OCCCC
Mol. weight [g/mol]: 262.37
CAS: 4121-12-4

Physical Properties

Property code	Value	Unit	Source
gf	-384.56	kJ/mol	Joback Method
hf	-738.74	kJ/mol	Joback Method
hfus	36.54	kJ/mol	Joback Method
hvap	67.44	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.406		Crippen Method
mcvol	211.170	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
tb	695.32	K	Joback Method
tc	887.08	K	Joback Method
tf	403.72	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.69	J/mol×K	695.32	Joback Method
cpg	589.11	J/mol×K	727.28	Joback Method
cpg	602.76	J/mol×K	759.24	Joback Method
cpg	615.62	J/mol×K	791.20	Joback Method
cpg	627.69	J/mol×K	823.16	Joback Method
cpg	638.97	J/mol×K	855.12	Joback Method

cpg	649.46	J/mol×K	887.08	Joback Method
hvapt	75.70	kJ/mol	340.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4121124&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume