Propionic acid, 3,3'-sulfonyldi-, didodecyl ester

Inchi: InChI=1S/C30H58O6S/c1-3-5-7-9-11-13-15-17-19-21-25-35-29(31)23-27-37(33,34)28-24

InchiKey: UMPQTYNTXDMGCO-UHFFFAOYSA-N

Formula: C30H58O6S

SMILES: CCCCCCCCCCCCOC(=O)CCS(=O)(=O)CCC(=O)OCCCCCCCCCCCC

Mol. weight [g/mol]: 546.84

CAS: 27326-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-734.66	kJ/mol	Joback Method
hf	-1605.48	kJ/mol	Joback Method
hfus	90.41	kJ/mol	Joback Method
hvap	119.32	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	8.110		Crippen Method
mcvol	476.530	ml/mol	McGowan Method
pc	674.30	kPa	Joback Method
tb	1086.16	K	Joback Method
tc	1389.37	K	Joback Method
tf	610.74	K	Joback Method
vc	1.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1697.34	J/mol×K	1086.16	Joback Method
cpg	1718.91	J/mol×K	1136.70	Joback Method
cpg	1736.63	J/mol×K	1187.23	Joback Method
cpg	1750.61	J/mol×K	1237.77	Joback Method
cpg	1760.97	J/mol×K	1288.30	Joback Method
cpg	1767.84	J/mol×K	1338.84	Joback Method
cpg	1771.33	J/mol×K	1389.37	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=C27326278&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume