DIBUTYL 3,3'-SULFONYLDIPROPIONATE

Other names: Dibutyl 3,3'-sulfonyldipropionate
Inchi: InChI=1S/C14H26O6S/c1-3-5-9-19-13(15)7-11-21(17,18)12-8-14(16)20-10-6-4-2/h3-12H
InchiKey: VUUQFLLRJFDANW-UHFFFAOYSA-N
Formula: C14H26O6S
SMILES: CCCCOC(=O)CCS(=O)(=O)CCC(=O)OCCCC
Mol. weight [g/mol]: 322.42

Physical Properties

Property code	Value	Unit	Source
af	0.9208		Cheméo Relay (1.0)
hf	-1237.26	kJ/mol	Cheméo Relay (1.0)
hfus	48.97	kJ/mol	Joback Method
hvap	110.31	kJ/mol	Cheméo Relay (1.0)
ie	9.66	eV	Cheméo Relay (1.0)
log10ws	-2.67		Cheméo Relay (1.0)
logp	1.868		Crippen Method
mcvol	251.090	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
tb	643.65	K	Cheméo Relay (1.0)
tc	813.90	K	Cheméo Relay (1.0)
tf	364.49	K	Cheméo Relay (1.0)
vc	0.928	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.15	J/mol×K	720.08	Joback Method
cpg	730.43	J/mol×K	749.42	Joback Method
cpg	744.87	J/mol×K	778.77	Joback Method
cpg	758.46	J/mol×K	808.11	Joback Method
cpg	771.18	J/mol×K	837.45	Joback Method
cpg	783.04	J/mol×K	866.80	Joback Method
cpg	794.03	J/mol×K	896.14	Joback Method
hfust	31.40	kJ/mol	344.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5423278&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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