HEXADECYL METHANESULFONATE

Inchi: InChI=1S/C17H36O3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-21(2,18)19/h3-17H
InchiKey: FESYLDKBOOCXRD-UHFFFAOYSA-N
Formula: C17H36O3S
SMILES: CCCCCCCCCCCCCCCCCOS(C)(=O)=O
Mol. weight [g/mol]: 320.54

Physical Properties

Property code	Value	Unit	Source
af	0.9635		Cheméo Relay (1.0)
gf	-481.28	kJ/mol	Joback Method
hf	-869.53	kJ/mol	Cheméo Relay (1.0)
hfus	52.35	kJ/mol	Joback Method
hvap	112.70	kJ/mol	Cheméo Relay (1.0)
ie	10.30	eV	Cheméo Relay (1.0)
log10ws	-6.73		Cheméo Relay (1.0)
logp	5.444		Crippen Method
mcvol	284.350	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
tb	628.98	K	Cheméo Relay (1.0)
tc	810.97	K	Cheméo Relay (1.0)
tf	313.52	K	Cheméo Relay (1.0)
vc	1.108	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.48	J/mol×K	658.56	Joback Method
cpg	818.62	J/mol×K	685.33	Joback Method
cpg	836.93	J/mol×K	712.10	Joback Method
cpg	854.43	J/mol×K	738.87	Joback Method
cpg	871.12	J/mol×K	765.64	Joback Method
cpg	887.01	J/mol×K	792.41	Joback Method
cpg	902.11	J/mol×K	819.18	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20779140&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

af:	Acentric Factor
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
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