Methanesulfonamide, N-heptyl-N-octyl-

Inchi: InChI=1S/C16H35NO2S/c1-4-6-8-10-12-14-16-17(20(3,18)19)15-13-11-9-7-5-2/h4-16H2
InchiKey: XEQDEIVUFVKGQP-UHFFFAOYSA-N
Formula: C16H35NO2S
SMILES: CCCCCCCCN(CCCCCCC)S(C)(=O)=O
Mol. weight [g/mol]: 305.52

Physical Properties

Property code	Value	Unit	Source
gf	-273.92	kJ/mol	Joback Method
hf	-759.39	kJ/mol	Joback Method
hfus	51.59	kJ/mol	Joback Method
hvap	71.89	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.579		Crippen Method
mcvol	274.370	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	625.70	K	Joback Method
tc	784.08	K	Joback Method
tf	341.11	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.65	J/mol×K	625.70	Joback Method
cpg	769.85	J/mol×K	652.10	Joback Method
cpg	788.22	J/mol×K	678.49	Joback Method
cpg	805.78	J/mol×K	704.89	Joback Method
cpg	822.55	J/mol×K	731.28	Joback Method
cpg	838.55	J/mol×K	757.68	Joback Method
cpg	853.78	J/mol×K	784.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308433&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
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