

Methanesulfonamide, N,N-diundecyl-

Inchi:	InChI=1S/C23H49NO2S/c1-4-6-8-10-12-14-16-18-20-22-24(27(3,25)26)23-21-19-17-15-
InchiKey:	MCOGYFFONVUHSB-UHFFFAOYSA-N
Formula:	C23H49NO2S
SMILES:	CCCCCCCCCCCN(CCCCCCCCCC)S(C)(=O)=O
Mol. weight [g/mol]:	403.71

Physical Properties

Property code	Value	Unit	Source
gf	-214.98	kJ/mol	Joback Method
hf	-903.87	kJ/mol	Joback Method
hfus	69.73	kJ/mol	Joback Method
hvap	87.47	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.310		Crippen Method
mvol	373.000	ml/mol	McGowan Method
pc	933.49	kPa	Joback Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tb	785.86	K	Joback Method
tc	962.14	K	Joback Method
tf	420.00	K	Joback Method
vc	1.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.27	J/mol×K	785.86	Joback Method
cpg	1198.63	J/mol×K	815.24	Joback Method
cpg	1219.79	J/mol×K	844.62	Joback Method
cpg	1239.78	J/mol×K	874.00	Joback Method
cpg	1258.65	J/mol×K	903.38	Joback Method
cpg	1276.42	J/mol×K	932.76	Joback Method
cpg	1293.14	J/mol×K	962.14	Joback Method

Sources

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=U308437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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