

2-Diethylaminoethyl isobutyl trisulfide

Other names:	Isobutyl 2-diethylaminoethyl trisulfide
Inchi:	InChI=1S/C10H23NS3/c1-5-11(6-2)7-8-12-14-13-9-10(3)4/h10H,5-9H2,1-4H3
InchiKey:	FKYPKOFUKOPYPJ-UHFFFAOYSA-N
Formula:	C10H23NS3
SMILES:	CCN(CC)CCSSSCC(C)C
Mol. weight [g/mol]:	253.49

Physical Properties

Property code	Value	Unit	Source
gf	241.02	kJ/mol	Joback Method
hf	-61.87	kJ/mol	Joback Method
hfus	33.54	kJ/mol	Joback Method
hvap	59.96	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	4.014		Crippen Method
mcvol	210.790	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1736.00		NIST Webbook
tb	646.54	K	Joback Method
tc	864.53	K	Joback Method
tf	323.13	K	Joback Method
vc	0.769	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.27	J/mol×K	646.54	Joback Method
cpg	548.12	J/mol×K	682.87	Joback Method
cpg	563.94	J/mol×K	719.20	Joback Method

cpg	578.76	J/mol×K	755.54	Joback Method
cpg	592.58	J/mol×K	791.87	Joback Method
cpg	605.43	J/mol×K	828.20	Joback Method
cpg	617.33	J/mol×K	864.53	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=R334844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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