2-Diethylaminoethyl isobutyl disulfide

Other names: Isobutyl 2-diethylaminoethyl disulfide
Inchi: InChI=1S/C10H23NS2/c1-5-11(6-2)7-8-12-13-9-10(3)4/h10H,5-9H2,1-4H3
InchiKey: LYLKVUMUXFAGGM-UHFFFAOYSA-N
Formula: C10H23NS2
SMILES: CCN(CC)CCSSCC(C)C
Mol. weight [g/mol]: 221.43

Physical Properties

Property code	Value	Unit	Source
gf	207.90	kJ/mol	Joback Method
hf	-103.74	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	53.14	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	3.366		Crippen Method
mcvol	194.440	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
tb	577.76	K	Joback Method
tc	779.22	K	Joback Method
tf	288.73	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.05	J/mol×K	577.76	Joback Method
cpg	489.06	J/mol×K	611.34	Joback Method
cpg	505.19	J/mol×K	644.91	Joback Method
cpg	520.46	J/mol×K	678.49	Joback Method

cpg	534.89	J/mol×K	712.07	Joback Method
cpg	548.50	J/mol×K	745.65	Joback Method
cpg	561.30	J/mol×K	779.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R334824&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