2-Diethylaminoethyl isobutyl sulfide

Other names: Isobutyl 2-diethylaminoethyl sulfide
Inchi: InChI=1S/C10H23NS/c1-5-11(6-2)7-8-12-9-10(3)4/h10H,5-9H2,1-4H3
InchiKey: ZBDCZOMEKJDMLI-UHFFFAOYSA-N
Formula: C10H23NS
SMILES: CCN(CC)CCSCC(C)C
Mol. weight [g/mol]: 189.36

Physical Properties

Property code	Value	Unit	Source
gf	174.78	kJ/mol	Joback Method
hf	-145.61	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	46.33	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.717		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1292.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1292.00		NIST Webbook
tb	508.98	K	Joback Method
tc	692.70	K	Joback Method
tf	254.33	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.83	J/mol×K	508.98	Joback Method
cpg	427.67	J/mol×K	539.60	Joback Method
cpg	443.75	J/mol×K	570.22	Joback Method
cpg	459.08	J/mol×K	600.84	Joback Method
cpg	473.70	J/mol×K	631.46	Joback Method

cpg	487.61	J/mol×K	662.08	Joback Method
cpg	500.84	J/mol×K	692.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R334839&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