Butyl 2-diethylaminoethyl sulfide

Other names: Butyl 2-diethylaminoethyl sulfide
Inchi: InChI=1S/C10H23NS/c1-4-7-9-12-10-8-11(5-2)6-3/h4-10H2,1-3H3
InchiKey: DMFWTLBQLIMYLP-UHFFFAOYSA-N
Formula: C10H23NS
SMILES: CCCCSCCN(CC)CC
Mol. weight [g/mol]: 189.37

Physical Properties

Property code	Value	Unit	Source
hf	-161.02	kJ/mol	Cheméo Relay (1.0)
hfus	28.81	kJ/mol	Joback Method
hvap	61.94	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	Cheméo Relay (1.0)
logp	2.862		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1335.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1337.00		NIST Webbook
tb	498.69	K	Cheméo Relay (1.0)
tc	673.75	K	Cheméo Relay (1.0)
tf	192.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.64	J/mol×K	509.42	Joback Method
cpg	427.07	J/mol×K	539.42	Joback Method
cpg	442.78	J/mol×K	569.42	Joback Method
cpg	457.78	J/mol×K	599.42	Joback Method
cpg	472.09	J/mol×K	629.42	Joback Method
cpg	485.74	J/mol×K	659.42	Joback Method

cpg	498.74	J/mol×K	689.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R334819&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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