

2-(Diisopropylamino)ethanethiol

Other names:	2-(diisopropylamino)ethane-1-thiol 2-[bis(1-methylethyl)amino]ethanethiol 2-diisopropyl aminoethanethiol Ethanethiol, 2-(diisopropylamino)- Ethanethiol, 2-[bis(1-methylethyl)amino]- USAF A-16784
Inchi:	InChI=1S/C8H19NS/c1-7(2)9(5-6-10)8(3)4/h7-8,10H,5-6H2,1-4H3
InchiKey:	IFZVKYXDCOHPOT-UHFFFAOYSA-N
Formula:	C8H19NS
SMILES:	CC(C)N(CCS)C(C)C
Mol. weight [g/mol]:	161.31
CAS:	5842-07-9

Physical Properties

Property code	Value	Unit	Source
gf	151.77	kJ/mol	Joback Method
hf	-113.00	kJ/mol	Joback Method
hfus	16.49	kJ/mol	Joback Method
hvap	41.41	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.035		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1113.40		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1113.50		NIST Webbook
tb	456.86	K	Joback Method
tc	648.72	K	Joback Method
tf	218.85	K	Joback Method
vc	0.543	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.54	J/molxK	456.86	Joback Method
cpg	332.17	J/molxK	488.84	Joback Method
cpg	347.04	J/molxK	520.81	Joback Method
cpg	361.18	J/molxK	552.79	Joback Method
cpg	374.63	J/molxK	584.77	Joback Method
cpg	387.39	J/molxK	616.75	Joback Method
cpg	399.50	J/molxK	648.72	Joback Method
pvap	9.28e-03	kPa	275.15	Vapor Pressure of 2-Dialkyl Aminoethanethiols
pvap	0.02	kPa	285.15	Vapor Pressure of 2-Dialkyl Aminoethanethiols
pvap	0.05	kPa	295.65	Vapor Pressure of 2-Dialkyl Aminoethanethiols

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.50 ± 0.50	K	2.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5842079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressure of 2-Dialkyl Aminoethanethiols:	https://www.doi.org/10.1021/je400136y
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
hvac:	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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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