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

Physical Properties

Property code	Value	Unit	Source
hfus	16.49	kJ/mol	Joback Method
logp	2.035		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
rinpol	1098.00		NIST Webbook
rinpol	1113.40		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1113.50		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
tb	461.81	K	Cheméo Relay (1.0)
tf	199.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.54	J/mol×K	456.86	Joback Method
cpg	332.17	J/mol×K	488.84	Joback Method
cpg	347.04	J/mol×K	520.81	Joback Method
cpg	361.18	J/mol×K	552.79	Joback Method
cpg	374.63	J/mol×K	584.77	Joback Method

cpg	387.39	J/mol×K	616.75	Joback Method
cpg	399.50	J/mol×K	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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Vapor Pressure of 2-Dialkyl Aminoethanethiols: https://www.doi.org/10.1021/je400136y

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5842079&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pvap: Vapor pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point