3-DIPROPYLAMINO-1,2-PROPANEDIOL

Other names: 1,2-Propanediol, 3-(dipropylamino)-
3-(dipropylamino)propane-1,2-diol
Inchi: InChI=1S/C9H21NO2/c1-3-5-10(6-4-2)7-9(12)8-11/h9,11-12H,3-8H2,1-2H3
InchiKey: CTSOJEIWXYRSEM-UHFFFAOYSA-N
Formula: C9H21NO2
SMILES: CCCN(CCC)CC(O)CO
Mol. weight [g/mol]: 175.27

Physical Properties

Property code	Value	Unit	Source
hf	-487.59	kJ/mol	Cheméo Relay (1.0)
hfus	26.74	kJ/mol	Joback Method
hvap	90.00	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-0.29		Cheméo Relay (1.0)
logp	0.462		Crippen Method
mcvol	159.390	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
tb	537.82	K	Cheméo Relay (1.0)
tc	694.54	K	Cheméo Relay (1.0)
tf	269.11	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.31	J/mol×K	601.68	Joback Method
cpg	440.93	J/mol×K	628.11	Joback Method
cpg	452.05	J/mol×K	654.54	Joback Method
cpg	462.69	J/mol×K	680.98	Joback Method
cpg	472.87	J/mol×K	707.41	Joback Method
cpg	482.60	J/mol×K	733.84	Joback Method
cpg	491.91	J/mol×K	760.27	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	1.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60302967&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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