3-(Diethylamino)-1,2-propanediol

Other names: 1,2-Propanediol, 3-(diethylamino)-
3-(diethylamino)propane-1,2-diol
Inchi: InChI=1S/C7H17NO2/c1-3-8(4-2)5-7(10)6-9/h7,9-10H,3-6H2,1-2H3
InchiKey: LTACQVCHVAUOKN-UHFFFAOYSA-N
Formula: C7H17NO2
SMILES: CCN(CC)CC(O)CO
Mol. weight [g/mol]: 147.22
CAS: 621-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-157.24	kJ/mol	Joback Method
hf	-430.02	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	0.04		Crippen Method
logp	-0.319		Crippen Method
mcvol	131.210	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	507.20	K	NIST Webbook
tc	714.63	K	Joback Method
tf	307.76	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.70	J/mol×K	555.92	Joback Method
cpg	343.87	J/mol×K	582.37	Joback Method
cpg	353.60	J/mol×K	608.82	Joback Method
cpg	362.91	J/mol×K	635.27	Joback Method
cpg	371.82	J/mol×K	661.72	Joback Method
cpg	380.34	J/mol×K	688.17	Joback Method
cpg	388.49	J/mol×K	714.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.84274e+01
Coeff. B	-5.86973e+03
Coeff. C	-8.21380e+01
Temperature range (K), min.	405.72
Temperature range (K), max.	529.66

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621567&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume