Propanol, 3-[[(1,4-benzodioxan-2-yl)methyl]amino]-

Inchi: InChI=1S/C12H17NO3/c14-7-3-6-13-8-10-9-15-11-4-1-2-5-12(11)16-10/h1-2,4-5,10,13-1
InchiKey: HCSGAGXOCHYBLF-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: OCCCNCC1COc2ccccc2O1
Mol. weight [g/mol]: 223.27
CAS: 74398-46-2

Physical Properties

Property code	Value	Unit	Source
gf	-18.08	kJ/mol	Joback Method
hf	-362.07	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	77.46	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	0.798		Crippen Method
mcvol	172.910	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	712.88	K	Joback Method
tc	917.75	K	Joback Method
tf	444.98	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.78	J/mol×K	712.88	Joback Method
cpg	518.87	J/mol×K	747.03	Joback Method
cpg	531.12	J/mol×K	781.17	Joback Method
cpg	542.58	J/mol×K	815.32	Joback Method
cpg	553.30	J/mol×K	849.46	Joback Method
cpg	563.33	J/mol×K	883.61	Joback Method
cpg	572.72	J/mol×K	917.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74398462&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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