Hexylcaine

Other names:	Cyclaine
	1-(Cyclohexylamino)-2-propanol benzoate (ester)
	2-Propanol, 1-(cyclohexylamino)-, benzoate (ester)
Inchi:	InChI=1S/C16H23NO2/c1-13(12-17-15-10-6-3-7-11-15)19-16(18)14-8-4-2-5-9-14/h2,4-5,
InchiKey:	DKLKMKYDWHYZTD-UHFFFAOYSA-N
Formula:	C16H23NO2
SMILES:	CC(CNC1CCCCC1)OC(=O)c1ccccc1
Mol. weight [g/mol]:	261.36
CAS:	532-77-4

Physical Properties

Property code	Value	Unit	Source
gf	73.73	kJ/mol	Joback Method
hf	-279.33	kJ/mol	Joback Method
hfus	27.43	kJ/mol	Joback Method
hvap	69.12	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.154		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	737.73	K	Joback Method
tc	966.49	K	Joback Method
tf	413.70	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.13	J/mol×K	737.73	Joback Method
cpg	672.20	J/mol×K	775.86	Joback Method
cpg	689.80	J/mol×K	813.98	Joback Method
cpg	705.98	J/mol×K	852.11	Joback Method

cpg	720.80	J/mol×K	890.24	Joback Method
cpg	734.29	J/mol×K	928.37	Joback Method
cpg	746.53	J/mol×K	966.49	Joback Method

Sources

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=C532774&Units=SI
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume