

Dicyclohexylcarbinol, formate

Inchi:	InChI=1S/C14H24O2/c15-11-16-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h11-14H,1-10H2
InchiKey:	UFZVWVJBGNATRO-UHFFFAOYSA-N
Formula:	C14H24O2
SMILES:	O=COC(C1CCCCC1)C1CCCCC1
Mol. weight [g/mol]:	224.34

Physical Properties

Property code	Value	Unit	Source
gf	-91.06	kJ/mol	Joback Method
hf	-446.73	kJ/mol	Joback Method
hfus	15.64	kJ/mol	Joback Method
hvap	56.36	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.689		Crippen Method
mcvol	193.840	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpola	1665.00		NIST Webbook
tb	629.46	K	Joback Method
tc	857.06	K	Joback Method
tf	311.53	K	Joback Method
vc	0.715	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.54	J/molxK	629.46	Joback Method
cpg	577.25	J/molxK	667.39	Joback Method
cpg	599.37	J/molxK	705.33	Joback Method
cpg	619.95	J/molxK	743.26	Joback Method
cpg	639.03	J/molxK	781.20	Joback Method
cpg	656.63	J/molxK	819.13	Joback Method
cpg	672.81	J/molxK	857.06	Joback Method
dvisc	0.0065955	Paxs	311.53	Joback Method
dvisc	0.0023302	Paxs	364.52	Joback Method

dvisc	0.0010721	Paxs	417.51	Joback Method
dvisc	0.0005875	Paxs	470.50	Joback Method
dvisc	0.0003636	Paxs	523.48	Joback Method
dvisc	0.0002458	Paxs	576.47	Joback Method
dvisc	0.0001775	Paxs	629.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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