

Cuparenal

Inchi:	InChI=1S/C15H20O/c1-14(2)9-4-10-15(14,3)13-7-5-12(11-16)6-8-13/h5-8,11H,4,9-10H2,
InchiKey:	KJYANGWERYBSJY-UHFFFAOYSA-N
Formula:	C15H20O
SMILES:	CC1(C)CCCC1(C)c1ccc(C=O)cc1
Mol. weight [g/mol]:	216.32
CAS:	16982-01-7

Physical Properties

Property code	Value	Unit	Source
gf	96.54	kJ/mol	Joback Method
hf	-142.83	kJ/mol	Joback Method
hfus	12.96	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.967		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook
tb	634.01	K	Joback Method
tc	874.13	K	Joback Method
tf	394.21	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.04	J/molxK	634.01	Joback Method
cpg	523.19	J/molxK	674.03	Joback Method
cpg	541.31	J/molxK	714.05	Joback Method
cpg	558.70	J/molxK	754.07	Joback Method
cpg	575.64	J/molxK	794.09	Joback Method
cpg	592.43	J/molxK	834.11	Joback Method
cpg	609.38	J/molxK	874.13	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=C16982017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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