

Cadinol

Inchi: InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h9-10,12-14,16H,5-
InchiKey: LHYHMMRYTDARSZ-XQLPTFJDSA-N
Formula: C15H26O
SMILES: CC1=CC2C(C(C)C)CCC(C)(O)C2CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	8.68	kJ/mol	Joback Method
hf	-368.61	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1633.00		NIST Webbook
ripol	2036.00		NIST Webbook
ripol	2036.00		NIST Webbook
tb	659.94	K	Joback Method
tc	865.11	K	Joback Method
tf	355.13	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.80	J/mol×K	659.94	Joback Method
cpg	617.79	J/mol×K	694.13	Joback Method
cpg	636.77	J/mol×K	728.33	Joback Method
cpg	654.86	J/mol×K	762.52	Joback Method

cpg	672.18	J/mol×K	796.72	Joback Method
cpg	688.83	J/mol×K	830.91	Joback Method
cpg	704.93	J/mol×K	865.11	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=R54901&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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