«gamma»-Cadinol

Inchi: InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h5,10,12-14,16H,6-9

InchiKey: INTCVZZCTDGTCB-VXGQWTEUSA-N

Formula: C15H26O

SMILES: CC1=CCC2C(C1)C(C(C)C)CCC2(C)O

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	1658.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1629.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2171.00		NIST Webbook
ripol	2137.00		NIST Webbook
ripol	2137.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2171.00		NIST Webbook
ripol	2137.00		NIST Webbook

ripol	2125.00		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

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=R609757&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
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