«beta»-Cadinol

Inchi: InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h10,12-14,16H,3,5-
InchiKey: DCGIIRVFKWJQME-VXGQWTEUSA-N
Formula: C15H26O
SMILES: C=C1CCC2C(C1)C(C(C)C)CCC2(C)O
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	41.43	kJ/mol	Joback Method
hf	-330.68	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1668.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1661.00		NIST Webbook
ripol	2201.00		NIST Webbook
ripol	2201.00		NIST Webbook
ripol	2165.00		NIST Webbook
ripol	2165.00		NIST Webbook
tb	654.96	K	Joback Method
tc	859.10	K	Joback Method
tf	355.53	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.74	J/mol×K	654.96	Joback Method
cpg	616.91	J/mol×K	688.98	Joback Method

cpg	636.06	J/mol×K	723.01	Joback Method
cpg	654.29	J/mol×K	757.03	Joback Method
cpg	671.72	J/mol×K	791.05	Joback Method
cpg	688.46	J/mol×K	825.08	Joback Method
cpg	704.61	J/mol×K	859.10	Joback Method

Sources

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=R234665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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