cadina-4,10(15)-dien-3-one

Inchi: InChI=1S/C15H22O/c1-9(2)12-6-5-10(3)13-8-15(16)11(4)7-14(12)13/h7,9,12-14H,3,5-6,8
InchiKey: QUTSKAAVYUOEQA-HSBZDZAISA-N
Formula: C15H22O
SMILES: C=C1CCC(C(C)C)C2C=C(C)C(=O)CC12
Mol. weight [g/mol]: 218.33
CAS: 39765-72-5

Physical Properties

Property code	Value	Unit	Source
gf	89.19	kJ/mol	Joback Method
hf	-264.74	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.760		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1743.00		NIST Webbook
ripol	2349.00		NIST Webbook
tb	639.17	K	Joback Method
tc	866.07	K	Joback Method
tf	356.55	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.23	J/mol×K	639.17	Joback Method
cpg	565.16	J/mol×K	676.99	Joback Method
cpg	585.76	J/mol×K	714.80	Joback Method
cpg	605.04	J/mol×K	752.62	Joback Method
cpg	623.01	J/mol×K	790.44	Joback Method
cpg	639.71	J/mol×K	828.25	Joback Method
cpg	655.13	J/mol×K	866.07	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=C39765725&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