(E)-15,16-Dinorlabda-8(17),11-dien-13-one

Inchi: InChI=1S/C18H28O/c1-13-7-10-16-17(3,4)11-6-12-18(16,5)15(13)9-8-14(2)19/h8-9,15-1
InchiKey: GWLGWWOKIBLQJF-CMDGGOBGSA-N
Formula: C18H28O
SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1C=CC(C)=O
Mol. weight [g/mol]: 260.41
CAS: 76497-69-3

Physical Properties

Property code	Value	Unit	Source
gf	151.76	kJ/mol	Joback Method
hf	-215.21	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	60.12	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.930		Crippen Method
mcvol	235.730	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	1994.10		NIST Webbook
rinpol	1994.10		NIST Webbook
tb	690.13	K	Joback Method
tc	917.31	K	Joback Method
tf	412.27	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.36	J/mol×K	690.13	Joback Method
cpg	715.27	J/mol×K	727.99	Joback Method
cpg	737.26	J/mol×K	765.86	Joback Method
cpg	758.59	J/mol×K	803.72	Joback Method
cpg	779.53	J/mol×K	841.58	Joback Method
cpg	800.37	J/mol×K	879.45	Joback Method
cpg	821.36	J/mol×K	917.31	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=C76497693&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume