

Eremophila ketone

Inchi:	InChI=1S/C15H24O/c1-10-5-6-11-13(2,3)12(16)14(4)7-8-15(10,11)9-14/h10-11H,5-9H2,
InchiKey:	FKIMAXRXZJXZBA-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1CCC2C(C)(C)C(=O)C3(C)CCC12C3
Mol. weight [g/mol]:	220.35
CAS:	158930-41-7

Physical Properties

Property code	Value	Unit	Source
gf	78.99	kJ/mol	Joback Method
hf	-279.51	kJ/mol	Joback Method
hfus	7.57	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.818		Crippen Method
mvol	191.200	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1566.60		NIST Webbook
tb	630.56	K	Joback Method
tc	875.45	K	Joback Method
tf	437.03	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.94	J/mol×K	630.56	Joback Method
cpg	584.99	J/mol×K	671.37	Joback Method
cpg	606.96	J/mol×K	712.19	Joback Method
cpg	628.30	J/mol×K	753.00	Joback Method
cpg	649.46	J/mol×K	793.82	Joback Method
cpg	670.93	J/mol×K	834.63	Joback Method
cpg	693.14	J/mol×K	875.45	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=C158930417&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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