

14-Oxocalamenene

Inchi:	InChI=1S/C15H20O/c1-10(2)13-7-5-12(9-16)14-6-4-11(3)8-15(13)14/h4,6,8-10,12-13H,5
InchiKey:	RXELGPYYZBYBFV-CHWSQXEVSAN
Formula:	C15H20O
SMILES:	<chem>Cc1ccc2c(c1)C(C(C)C)CCC2C=O</chem>
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	107.55	kJ/mol	Joback Method
hf	-183.90	kJ/mol	Joback Method
hfus	23.74	kJ/mol	Joback Method
hvap	58.69	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.811		Crippen Method
mvol	189.160	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
ripol	2495.00		NIST Webbook
ripol	2495.00		NIST Webbook
tb	633.80	K	Joback Method
tc	854.49	K	Joback Method
tf	347.45	K	Joback Method
vc	0.727	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.06	J/molxK	633.80	Joback Method
cpg	526.79	J/molxK	670.58	Joback Method
cpg	544.34	J/molxK	707.36	Joback Method
cpg	560.76	J/molxK	744.14	Joback Method
cpg	576.09	J/molxK	780.93	Joback Method
cpg	590.40	J/molxK	817.71	Joback Method
cpg	603.75	J/molxK	854.49	Joback Method
dvisc	0.0021706	Paxs	347.45	Joback Method

dvisc	0.0013652	Paxs	395.17	Joback Method
dvisc	0.0009489	Paxs	442.90	Joback Method
dvisc	0.0007079	Paxs	490.62	Joback Method
dvisc	0.0005563	Paxs	538.35	Joback Method
dvisc	0.0004546	Paxs	586.07	Joback Method
dvisc	0.0003830	Paxs	633.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R407204&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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