

Carquejyl acetate

Inchi:	InChI=1S/C12H16O2/c1-8(2)12-9(3)6-5-7-11(12)14-10(4)13/h5,7,11-12H,1,3,6H2,2,4H3
InchiKey:	LCKQEGQKVDFBIO-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	<chem>C=C(C)C1C(=C)CC=CC1OC(C)=O</chem>
Mol. weight [g/mol]:	192.25

Physical Properties

Property code	Value	Unit	Source
gf	-4.69	kJ/mol	Joback Method
hf	-244.17	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.626		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
ripol	1293.00		NIST Webbook
ripol	1289.00		NIST Webbook
ripol	1736.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1669.00		NIST Webbook
tb	560.01	K	Joback Method
tc	770.57	K	Joback Method
tf	299.02	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.25	J/molxK	560.01	Joback Method
cpg	412.24	J/molxK	595.10	Joback Method
cpg	428.33	J/molxK	630.20	Joback Method
cpg	443.52	J/molxK	665.29	Joback Method
cpg	457.83	J/molxK	700.38	Joback Method

cpg	471.26	J/mol×K	735.48	Joback Method
cpg	483.84	J/mol×K	770.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R485373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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