

Iridomyrmecin

Other names:	Cyclopenta[c]pyran-3(1H)-one, hexahydro-4,7-dimethyl-, [4S-(4«alpha»,4a«beta»,7«beta»,7a«beta»)]-Cyclopenta[c]pyran-3(1H)-one, hexahydro-4,7-dimethyl-, Cyclopenta[c]pyran-3(1H)-one, hexahydro-4,7-dimethyl-, (4«alpha»,4a«beta»,7«beta»,7a«beta»)-(-)-Iridomyrmecina Iridomyrmexin Isoiridomyrmecin
Inchi:	InChI=1S/C10H16O2/c1-6-3-4-8-7(2)10(11)12-5-9(6)8/h6-9H,3-5H2,1-2H3/t6-,7-,8+,9+/m
InchiKey:	LYEFRAMOOLOUKA-RBXMUDONSA-N
Formula:	C10H16O2
SMILES:	CC1CCC2C(C)C(=O)OCC12
Mol. weight [g/mol]:	168.23
CAS:	485-43-8

Physical Properties

Property code	Value	Unit	Source
gf	-105.61	kJ/mol	Joback Method
hf	-432.99	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	46.34	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.842		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1463.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1400.00		NIST Webbook
tb	539.92	K	Joback Method
tc	767.98	K	Joback Method
tf	314.09	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	358.98	J/mol×K	539.92	Joback Method
cpg	379.23	J/mol×K	577.93	Joback Method
cpg	398.36	J/mol×K	615.94	Joback Method
cpg	416.39	J/mol×K	653.95	Joback Method
cpg	433.33	J/mol×K	691.96	Joback Method
cpg	449.20	J/mol×K	729.97	Joback Method
cpg	464.00	J/mol×K	767.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C485438&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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