

Actinidiolide

Inchi: InChI=1S/C11H14O2/c1-10(2)5-4-6-11(3)8(10)7-9(12)13-11/h4,6-7H,5H2,1-3H3/t11-/m0
InchiKey: VGQSMHFBCKKQHB-NSHDSACASA-N
Formula: C11H14O2
SMILES: CC1(C)CC=CC2(C)OC(=O)C=C12
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	-42.46	kJ/mol	Joback Method
hf	-278.38	kJ/mol	Joback Method
hfus	11.16	kJ/mol	Joback Method
hvap	48.12	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.214		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	575.92	K	Joback Method
tc	825.11	K	Joback Method
tf	395.68	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.29	J/molxK	575.92	Joback Method
cpg	380.82	J/molxK	617.45	Joback Method
cpg	396.25	J/molxK	658.98	Joback Method
cpg	410.88	J/molxK	700.52	Joback Method
cpg	425.00	J/molxK	742.05	Joback Method
cpg	438.90	J/molxK	783.58	Joback Method
cpg	452.88	J/molxK	825.11	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=R432809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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