

Neocurdione

Inchi:	InChI=1S/C15H24O2/c1-10(2)13-9-14(16)12(4)7-5-6-11(3)8-15(13)17/h6,10,12-13H,5,7-
InchiKey:	KDPFMRXIVDLQKX-IZZDOVSWSA-N
Formula:	C15H24O2
SMILES:	CC1=CCCC(C)C(=O)CC(C(C)C)C(=O)C1
Mol. weight [g/mol]:	236.35
CAS:	108944-67-8

Physical Properties

Property code	Value	Unit	Source
gf	-183.53	kJ/mol	Joback Method
hf	-577.96	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.553		Crippen Method
mvol	210.190	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1761.70		NIST Webbook
rinpol	1747.00		NIST Webbook
tb	713.90	K	Joback Method
tc	956.91	K	Joback Method
tf	382.59	K	Joback Method
vc	0.769	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.90	J/molxK	713.90	Joback Method
cpg	654.71	J/molxK	754.40	Joback Method
cpg	676.68	J/molxK	794.90	Joback Method
cpg	696.72	J/molxK	835.40	Joback Method
cpg	714.74	J/molxK	875.90	Joback Method
cpg	730.66	J/molxK	916.41	Joback Method
cpg	744.39	J/molxK	956.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108944678&Units=SI

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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