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: C/C1=C\CCC(C)C(=O)CC(C(C)C)C(=O)C1
Mol. weight [g/mol]: 236.36

Physical Properties

Property code	Value	Unit	Source
hfus	15.44	kJ/mol	Joback Method
logp	3.553		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
rinpol	1761.70		NIST Webbook
rinpol	1747.00		NIST Webbook

Temperature Dependent Properties

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

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices