

2,6-Dicyclohexyl-4-isopropylphenyl acetate

Inchi:	InChI=1S/C23H34O2/c1-16(2)20-14-21(18-10-6-4-7-11-18)23(25-17(3)24)22(15-20)19-1
InchiKey:	PINPBOZUOFWMBF-UHFFFAOYSA-N
Formula:	C23H34O2
SMILES:	CC(=O)Oc1c(C2CCCCC2)cc(C(C)C)cc1C1CCCCC1
Mol. weight [g/mol]:	342.51
CAS:	116659-39-3

Physical Properties

Property code	Value	Unit	Source
gf	38.84	kJ/mol	Joback Method
hf	-457.37	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	80.68	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.831		Crippen Method
mcvol	296.890	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
tb	882.21	K	Joback Method
tc	1120.17	K	Joback Method
tf	484.87	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.88	J/molxK	882.21	Joback Method
cpg	1020.86	J/molxK	921.87	Joback Method
cpg	1039.87	J/molxK	961.53	Joback Method
cpg	1056.97	J/molxK	1001.19	Joback Method
cpg	1072.21	J/molxK	1040.85	Joback Method
cpg	1085.67	J/molxK	1080.51	Joback Method
cpg	1097.41	J/molxK	1120.17	Joback Method
dvisc	0.0008276	Paxs	484.87	Joback Method
dvisc	0.0003925	Paxs	551.09	Joback Method

dvisc	0.0002184	Paxs	617.32	Joback Method
dvisc	0.0001362	Paxs	683.54	Joback Method
dvisc	0.0000923	Paxs	749.76	Joback Method
dvisc	0.0000666	Paxs	815.99	Joback Method
dvisc	0.0000505	Paxs	882.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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