

1,2-Cyclohexanedicarboxylic acid, isohexyl 4-isopropylphenyl ester

Inchi: InChI=1S/C23H34O4/c1-16(2)8-7-15-26-22(24)20-9-5-6-10-21(20)23(25)27-19-13-11-18
InchiKey: ACMVKMVHPOYRJX-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-210.42	kJ/mol	Joback Method
hf	-759.17	kJ/mol	Joback Method
hfus	40.41	kJ/mol	Joback Method
hvap	87.39	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.501		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
rinpol	2647.00		NIST Webbook
tb	923.88	K	Joback Method
tc	1145.45	K	Joback Method
tf	505.37	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.54	J/molxK	923.88	Joback Method
cpg	1075.78	J/molxK	960.81	Joback Method
cpg	1091.31	J/molxK	997.74	Joback Method
cpg	1105.15	J/molxK	1034.67	Joback Method
cpg	1117.34	J/molxK	1071.59	Joback Method
cpg	1127.91	J/molxK	1108.52	Joback Method
cpg	1136.91	J/molxK	1145.45	Joback Method

dvisc	0.0006795	Paxs	505.37	Joback Method
dvisc	0.0003193	Paxs	575.12	Joback Method
dvisc	0.0001767	Paxs	644.87	Joback Method
dvisc	0.0001097	Paxs	714.62	Joback Method
dvisc	0.0000742	Paxs	784.38	Joback Method
dvisc	0.0000534	Paxs	854.13	Joback Method
dvisc	0.0000405	Paxs	923.88	Joback Method

Sources

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=U339607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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