

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

Inchi: InChI=1S/C25H38O4/c1-4-5-6-7-8-11-18-28-24(26)22-12-9-10-13-23(22)25(27)29-21-16
InchiKey: YQKUSWBUJLAWJU-UHFFFAOYSA-N
Formula: C25H38O4
SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-191.14	kJ/mol	Joback Method
hf	-795.17	kJ/mol	Joback Method
hfus	49.11	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.425		Crippen Method
mcvol	343.370	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
rinpol	2887.00		NIST Webbook
rinpol	2851.00		NIST Webbook
rinpol	2851.00		NIST Webbook
tb	970.08	K	Joback Method
tc	1192.24	K	Joback Method
tf	542.91	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.09	J/molxK	970.08	Joback Method
cpg	1248.08	J/molxK	1155.22	Joback Method
cpg	1238.06	J/molxK	1118.19	Joback Method
cpg	1226.39	J/molxK	1081.16	Joback Method
cpg	1213.03	J/molxK	1044.13	Joback Method
cpg	1197.94	J/molxK	1007.11	Joback Method
cpg	1256.51	J/molxK	1192.24	Joback Method

dvisc	0.0000332	Paxs	970.08	Joback Method
dvisc	0.0000434	Paxs	898.88	Joback Method
dvisc	0.0000595	Paxs	827.69	Joback Method
dvisc	0.0000866	Paxs	756.50	Joback Method
dvisc	0.0001362	Paxs	685.30	Joback Method
dvisc	0.0002380	Paxs	614.11	Joback Method
dvisc	0.0004812	Paxs	542.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339610&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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