

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

Inchi: InChI=1S/C22H32O4/c1-4-5-8-15-25-21(23)19-9-6-7-10-20(19)22(24)26-18-13-11-17(12)
InchiKey: ZMUSWWIRYNGVBR-UHFFFAOYSA-N
Formula: C22H32O4
SMILES: CCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-216.40	kJ/mol	Joback Method
hf	-733.25	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.255		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	901.44	K	Joback Method
tc	1121.08	K	Joback Method
tf	509.10	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.28	J/molxK	901.44	Joback Method
cpg	1014.56	J/molxK	938.05	Joback Method
cpg	1030.19	J/molxK	974.65	Joback Method
cpg	1044.22	J/molxK	1011.26	Joback Method
cpg	1056.66	J/molxK	1047.87	Joback Method
cpg	1067.56	J/molxK	1084.47	Joback Method
cpg	1076.93	J/molxK	1121.08	Joback Method

dvisc	0.0006727	Paxs	509.10	Joback Method
dvisc	0.0003428	Paxs	574.49	Joback Method
dvisc	0.0002005	Paxs	639.88	Joback Method
dvisc	0.0001295	Paxs	705.27	Joback Method
dvisc	0.0000901	Paxs	770.66	Joback Method
dvisc	0.0000664	Paxs	836.05	Joback Method
dvisc	0.0000511	Paxs	901.44	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=U339606&Units=SI

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
mvol:	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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