

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

Inchi:	InChI=1S/C20H28O4/c1-4-13-23-19(21)17-7-5-6-8-18(17)20(22)24-16-11-9-15(10-12-16
InchiKey:	FSCUPDWJGYOUJJ-UHFFFAOYSA-N
Formula:	C20H28O4
SMILES:	CCCOC(=O)C1CCCCC1C(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-233.24	kJ/mol	Joback Method
hf	-691.97	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.475		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	2404.00		NIST Webbook
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	855.68	K	Joback Method
tc	1077.51	K	Joback Method
tf	486.56	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.32	J/molxK	855.68	Joback Method
cpg	894.86	J/molxK	892.65	Joback Method
cpg	910.82	J/molxK	929.62	Joback Method
cpg	925.22	J/molxK	966.60	Joback Method
cpg	938.07	J/molxK	1003.57	Joback Method
cpg	949.40	J/molxK	1040.54	Joback Method
cpg	959.24	J/molxK	1077.51	Joback Method

dvisc	0.0008252	Paxs	486.56	Joback Method
dvisc	0.0004299	Paxs	548.08	Joback Method
dvisc	0.0002555	Paxs	609.60	Joback Method
dvisc	0.0001670	Paxs	671.12	Joback Method
dvisc	0.0001172	Paxs	732.64	Joback Method
dvisc	0.0000870	Paxs	794.16	Joback Method
dvisc	0.0000673	Paxs	855.68	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=U339603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvac:	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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