

1,2-Cyclohexanedicarboxylic acid, 3-methylphenyl pentyl ester

Inchi:	InChI=1S/C20H28O4/c1-3-4-7-13-23-19(21)17-11-5-6-12-18(17)20(22)24-16-10-8-9-15(2)
InchiKey:	CUROEOYOEU TLPP-UHFFFAOYSA-N
Formula:	C20H28O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-230.80	kJ/mol	Joback Method
hf	-686.69	kJ/mol	Joback Method
hfus	39.69	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.440		Crippen Method
mvol	272.920	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	2422.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	856.12	K	Joback Method
tc	1075.16	K	Joback Method
tf	501.56	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.81	J/molxK	856.12	Joback Method
cpg	894.16	J/molxK	892.63	Joback Method
cpg	909.97	J/molxK	929.13	Joback Method
cpg	924.26	J/molxK	965.64	Joback Method
cpg	937.07	J/molxK	1002.15	Joback Method
cpg	948.40	J/molxK	1038.65	Joback Method
cpg	958.29	J/molxK	1075.16	Joback Method
dvisc	0.0007355	Paxs	501.56	Joback Method

dvisc	0.0004093	Paxs	560.65	Joback Method
dvisc	0.0002547	Paxs	619.75	Joback Method
dvisc	0.0001721	Paxs	678.84	Joback Method
dvisc	0.0001239	Paxs	737.93	Joback Method
dvisc	0.0000936	Paxs	797.03	Joback Method
dvisc	0.0000735	Paxs	856.12	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=U339831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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