

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

Inchi: InChI=1S/C23H34O4/c1-3-4-5-6-7-10-16-26-22(24)20-14-8-9-15-21(20)23(25)27-19-13-12
InchiKey: GUUSMKUJTLUXQV-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-205.54	kJ/mol	Joback Method
hf	-748.61	kJ/mol	Joback Method
hfus	47.46	kJ/mol	Joback Method
hvap	88.16	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.611		Crippen Method
mvol	315.190	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinpol	2723.00		NIST Webbook
rinpol	2723.00		NIST Webbook
tb	924.76	K	Joback Method
tc	1142.66	K	Joback Method
tf	535.37	K	Joback Method
vc	1.196	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.65	J/molxK	924.76	Joback Method
cpg	1074.69	J/molxK	961.08	Joback Method
cpg	1090.08	J/molxK	997.39	Joback Method
cpg	1103.88	J/molxK	1033.71	Joback Method
cpg	1116.10	J/molxK	1070.02	Joback Method
cpg	1126.79	J/molxK	1106.34	Joback Method
cpg	1135.97	J/molxK	1142.66	Joback Method
dvisc	0.0005441	Paxs	535.37	Joback Method

dvisc	0.0002926	Paxs	600.27	Joback Method
dvisc	0.0001776	Paxs	665.17	Joback Method
dvisc	0.0001178	Paxs	730.06	Joback Method
dvisc	0.0000836	Paxs	794.96	Joback Method
dvisc	0.0000624	Paxs	859.86	Joback Method
dvisc	0.0000486	Paxs	924.76	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=U339835&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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