

Isophthalic acid, di(3,5-dimethylcyclohexyl) ester

Inchi:	InChI=1S/C24H34O4/c1-15-8-16(2)11-21(10-15)27-23(25)19-6-5-7-20(14-19)24(26)28-2
InchiKey:	MKWXLHXKXJQDCI-UHFFFAOYSA-N
Formula:	C24H34O4
SMILES:	CC1CC(C)CC(OC(=O)c2ccccc(C(=O)OC3CC(C)CC(C)C3)c2)C1
Mol. weight [g/mol]:	386.52

Physical Properties

Property code	Value	Unit	Source
gf	-195.80	kJ/mol	Joback Method
hf	-775.95	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	89.89	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.650		Crippen Method
mcvol	318.420	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinpol	2975.00		NIST Webbook
tb	953.18	K	Joback Method
tc	1188.58	K	Joback Method
tf	541.30	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.96	J/molxK	953.18	Joback Method
cpg	1144.63	J/molxK	992.41	Joback Method
cpg	1159.93	J/molxK	1031.65	Joback Method
cpg	1172.90	J/molxK	1070.88	Joback Method
cpg	1183.54	J/molxK	1110.12	Joback Method
cpg	1191.88	J/molxK	1149.35	Joback Method
cpg	1197.94	J/molxK	1188.58	Joback Method
dvisc	0.0007818	Paxs	541.30	Joback Method
dvisc	0.0004604	Paxs	609.95	Joback Method

dvisc	0.0003018	Paxs	678.59	Joback Method
dvisc	0.0002138	Paxs	747.24	Joback Method
dvisc	0.0001605	Paxs	815.89	Joback Method
dvisc	0.0001260	Paxs	884.53	Joback Method
dvisc	0.0001024	Paxs	953.18	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=U343822&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
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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