Isophthalic acid, di(3,4-dimethylcyclohexyl) ester

Inchi: InChI=1S/C24H34O4/c1-15-8-10-21(12-17(15)3)27-23(25)19-6-5-7-20(14-19)24(26)28-2
InchiKey: KUNRZTCFBZTQPL-UHFFFAOYSA-N
Formula: C24H34O4
SMILES: CC1CCC(OC(=O)c2cccc(C(=O)OC3CCC(C)C(C)C3)c2)CC1C
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	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
tb	953.18	K	Joback Method
tc	1188.58	K	Joback Method
tf	541.30	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.96	J/mol×K	953.18	Joback Method
cpg	1144.63	J/mol×K	992.41	Joback Method
cpg	1159.93	J/mol×K	1031.65	Joback Method
cpg	1172.90	J/mol×K	1070.88	Joback Method
cpg	1183.54	J/mol×K	1110.12	Joback Method
cpg	1191.88	J/mol×K	1149.35	Joback Method
cpg	1197.94	J/mol×K	1188.58	Joback Method
dvisc	0.0007818	Pa×s	541.30	Joback Method

dvisc	0.0004604	Pa×s	609.95	Joback Method
dvisc	0.0003018	Pa×s	678.59	Joback Method
dvisc	0.0002138	Pa×s	747.24	Joback Method
dvisc	0.0001605	Pa×s	815.89	Joback Method
dvisc	0.0001260	Pa×s	884.53	Joback Method
dvisc	0.0001024	Pa×s	953.18	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=U343807&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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