Isophthalic acid, cyclohexylmethyl isohexyl ester

Inchi: InChI=1S/C21H30O4/c1-16(2)8-7-13-24-20(22)18-11-6-12-19(14-18)21(23)25-15-17-9-4

InchiKey: IVBSYEGRIRVRNW-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-217.11	kJ/mol	Joback Method
hf	-692.27	kJ/mol	Joback Method
hfus	37.68	kJ/mol	Joback Method
hvap	83.63	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.017		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	2710.00		NIST Webbook
rinpol	2710.00		NIST Webbook
tb	883.23	K	Joback Method
tc	1103.85	K	Joback Method
tf	502.07	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.97	J/mol×K	883.23	Joback Method
cpg	950.02	J/mol×K	920.00	Joback Method
cpg	965.53	J/mol×K	956.77	Joback Method
cpg	979.52	J/mol×K	993.54	Joback Method
cpg	992.03	J/mol×K	1030.31	Joback Method
cpg	1003.09	J/mol×K	1067.08	Joback Method
cpg	1012.74	J/mol×K	1103.85	Joback Method
dvisc	0.0006857	Pa×s	502.07	Joback Method

dvisc	0.0003375	Pa×s	565.60	Joback Method
dvisc	0.0001917	Pa×s	629.12	Joback Method
dvisc	0.0001208	Pa×s	692.65	Joback Method
dvisc	0.0000822	Pa×s	756.18	Joback Method
dvisc	0.0000594	Pa×s	819.70	Joback Method
dvisc	0.0000450	Pa×s	883.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U343828&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