Isophthalic acid, 2-methylcyclohexyl octyl ester

Inchi: InChI=1S/C23H34O4/c1-3-4-5-6-7-10-16-26-22(24)19-13-11-14-20(17-19)23(25)27-21-1

InchiKey: JWAZXWZYRDGVLZ-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)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	-7.16		Crippen Method
logp	5.939		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinpol	2871.00		NIST Webbook
rinpol	2871.00		NIST Webbook
tb	924.76	K	Joback Method
tc	1142.66	K	Joback Method
tf	535.37	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002926	Pa×s	600.27	Joback Method
dvisc	0.0001776	Pa×s	665.17	Joback Method
dvisc	0.0001178	Pa×s	730.06	Joback Method
dvisc	0.0000836	Pa×s	794.96	Joback Method
dvisc	0.0000624	Pa×s	859.86	Joback Method
dvisc	0.0000486	Pa×s	924.76	Joback Method

Sources

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=U345752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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