Isophthalic acid, dodecyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C27H42O4/c1-3-4-5-6-7-8-9-10-11-14-20-30-26(28)23-17-15-18-24(21-23)27(2

InchiKey: NNZHRAQAXMEBKY-UHFFFAOYSA-N

Formula: C27H42O4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1

Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-171.86	kJ/mol	Joback Method
hf	-831.17	kJ/mol	Joback Method
hfus	57.82	kJ/mol	Joback Method
hvap	97.07	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	7.500		Crippen Method
mcvol	371.550	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	3299.00		NIST Webbook
tb	1016.28	K	Joback Method
tc	1244.40	K	Joback Method
tf	580.45	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1305.23	J/mol×K	1016.28	Joback Method
cpg	1321.91	J/mol×K	1054.30	Joback Method
cpg	1336.69	J/mol×K	1092.32	Joback Method
cpg	1349.64	J/mol×K	1130.34	Joback Method
cpg	1360.79	J/mol×K	1168.36	Joback Method
cpg	1370.22	J/mol×K	1206.38	Joback Method
cpg	1377.97	J/mol×K	1244.40	Joback Method
dvisc	0.0003459	Pa×s	580.45	Joback Method
dvisc	0.0001786	Pa×s	653.09	Joback Method

dvisc	0.0001053	Pa×s	725.73	Joback Method
dvisc	0.0000684	Pa×s	798.37	Joback Method
dvisc	0.0000477	Pa×s	871.00	Joback Method
dvisc	0.0000352	Pa×s	943.64	Joback Method
dvisc	0.0000271	Pa×s	1016.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345756&Units=SI
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

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