Isophthalic acid, cyclopentylmethyl dodecyl ester

Inchi: InChI=1S/C26H40O4/c1-2-3-4-5-6-7-8-9-10-13-19-29-25(27)23-17-14-18-24(20-23)26(28

InchiKey: TZXNHISFKFEFQT-UHFFFAOYSA-N

Formula: C26H40O4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCC2)c1

Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-160.47	kJ/mol	Joback Method
hf	-784.03	kJ/mol	Joback Method
hfus	56.26	kJ/mol	Joback Method
hvap	94.98	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.111		Crippen Method
mcvol	357.460	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rinpol	3435.00		NIST Webbook
rinpol	3435.00		NIST Webbook
tb	993.80	K	Joback Method
tc	1217.19	K	Joback Method
tf	576.94	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1234.52	J/mol×K	993.80	Joback Method
cpg	1251.52	J/mol×K	1031.03	Joback Method
cpg	1266.93	J/mol×K	1068.26	Joback Method
cpg	1280.83	J/mol×K	1105.50	Joback Method
cpg	1293.27	J/mol×K	1142.73	Joback Method
cpg	1304.33	J/mol×K	1179.96	Joback Method
cpg	1314.06	J/mol×K	1217.19	Joback Method
dvisc	0.0004093	Pa×s	576.94	Joback Method

dvisc	0.0002177	Pa×s	646.42	Joback Method
dvisc	0.0001309	Pa×s	715.89	Joback Method
dvisc	0.0000861	Pa×s	785.37	Joback Method
dvisc	0.0000607	Pa×s	854.85	Joback Method
dvisc	0.0000450	Pa×s	924.32	Joback Method
dvisc	0.0000348	Pa×s	993.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345770&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