Isophthalic acid, cyclopentylmethyl tetradecyl ester

Inchi: InChI=1S/C28H44O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-21-31-27(29)25-19-16-20-26(22-25
InchiKey: QUYCSQDKMDCPNM-UHFFFAOYSA-N
Formula: C28H44O4
SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCC2)c1
Mol. weight [g/mol]: 444.65

Physical Properties

Property code	Value	Unit	Source
gf	-143.63	kJ/mol	Joback Method
hf	-825.31	kJ/mol	Joback Method
hfus	61.44	kJ/mol	Joback Method
hvap	99.43	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	7.891		Crippen Method
mcvol	385.640	ml/mol	McGowan Method
pc	908.34	kPa	Joback Method
rinpol	3607.00		NIST Webbook
rinpol	3607.00		NIST Webbook
tb	1039.56	K	Joback Method
tc	1273.30	K	Joback Method
tf	599.48	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1360.04	J/mol×K	1039.56	Joback Method
cpg	1377.31	J/mol×K	1078.52	Joback Method
cpg	1392.84	J/mol×K	1117.47	Joback Method
cpg	1406.71	J/mol×K	1156.43	Joback Method
cpg	1419.00	J/mol×K	1195.39	Joback Method
cpg	1429.81	J/mol×K	1234.34	Joback Method
cpg	1439.21	J/mol×K	1273.30	Joback Method
dvisc	0.0003221	Pa×s	599.48	Joback Method

dvisc	0.0001681	Pa×s	672.83	Joback Method
dvisc	0.0000997	Pa×s	746.17	Joback Method
dvisc	0.0000649	Pa×s	819.52	Joback Method
dvisc	0.0000454	Pa×s	892.87	Joback Method
dvisc	0.0000335	Pa×s	966.21	Joback Method
dvisc	0.0000258	Pa×s	1039.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345771&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