Isophthalic acid, 3-methylbutyl pentadecyl ester

Inchi: InChI=1S/C28H46O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-21-31-27(29)25-18-17-19-26

InchiKey: ZJXCOBBTRFKDCO-UHFFFAOYSA-N

Formula: C28H46O4

SMILES: CCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)c1

Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-182.62	kJ/mol	Joback Method
hf	-891.07	kJ/mol	Joback Method
hfus	63.98	kJ/mol	Joback Method
hvap	98.78	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.137		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	821.01	kPa	Joback Method
rinpol	3242.00		NIST Webbook
tb	1023.84	K	Joback Method
tc	1257.25	K	Joback Method
tf	573.58	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.87	J/mol×K	1023.84	Joback Method
cpg	1443.15	J/mol×K	1218.35	Joback Method
cpg	1431.78	J/mol×K	1179.45	Joback Method
cpg	1418.83	J/mol×K	1140.55	Joback Method
cpg	1404.24	J/mol×K	1101.64	Joback Method
cpg	1387.95	J/mol×K	1062.74	Joback Method
cpg	1453.02	J/mol×K	1257.25	Joback Method
dvisc	0.0000152	Pa×s	1023.84	Joback Method
dvisc	0.0000203	Pa×s	948.80	Joback Method

dvisc	0.0000283	Pa×s	873.75	Joback Method
dvisc	0.0000422	Pa×s	798.71	Joback Method
dvisc	0.0000682	Pa×s	723.67	Joback Method
dvisc	0.0001234	Pa×s	648.62	Joback Method
dvisc	0.0002604	Pa×s	573.58	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=U356470&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