Isophthalic acid, hexyl pentadecyl ester

Inchi: InChI=1S/C29H48O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-19-24-33-29(31)27-22-20-21-
InchiKey: XTQSJSDBMMDVHI-UHFFFAOYSA-N
Formula: C29H48O4
SMILES: CCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCC)c1
Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-171.76	kJ/mol	Joback Method
hf	-906.43	kJ/mol	Joback Method
hfus	70.09	kJ/mol	Joback Method
hvap	101.40	kJ/mol	Joback Method
log10ws	-9.91		Crippen Method
logp	8.672		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	774.18	kPa	Joback Method
rinpol	3478.00		NIST Webbook
rinpol	3478.00		NIST Webbook
tb	1047.16	K	Joback Method
tc	1291.10	K	Joback Method
tf	599.85	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.07	J/mol×K	1047.16	Joback Method
cpg	1507.75	J/mol×K	1250.44	Joback Method
cpg	1496.34	J/mol×K	1209.79	Joback Method
cpg	1483.25	J/mol×K	1169.13	Joback Method
cpg	1468.40	J/mol×K	1128.47	Joback Method
cpg	1451.70	J/mol×K	1087.82	Joback Method
cpg	1517.56	J/mol×K	1291.10	Joback Method
dvisc	0.0000143	Pa×s	1047.16	Joback Method

dvisc	0.0000189	Pa×s	972.61	Joback Method
dvisc	0.0000260	Pa×s	898.06	Joback Method
dvisc	0.0000380	Pa×s	823.50	Joback Method
dvisc	0.0000598	Pa×s	748.95	Joback Method
dvisc	0.0001042	Pa×s	674.40	Joback Method
dvisc	0.0002083	Pa×s	599.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344714&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

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

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