Isophthalic acid, pent-4-enyl tetradecyl ester

Inchi: InChI=1S/C27H42O4/c1-3-5-7-8-9-10-11-12-13-14-15-17-22-31-27(29)25-20-18-19-24(2
InchiKey: WJUAVPVNYRLUJA-UHFFFAOYSA-N
Formula: C27H42O4
SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCCC)c1
Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-100.76	kJ/mol	Joback Method
hf	-739.72	kJ/mol	Joback Method
hfus	63.63	kJ/mol	Joback Method
hvap	96.28	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.668		Crippen Method
mcvol	378.110	ml/mol	McGowan Method
pc	885.77	kPa	Joback Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
tb	998.08	K	Joback Method
tc	1223.21	K	Joback Method
tf	575.55	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1276.31	J/mol×K	998.08	Joback Method
cpg	1348.69	J/mol×K	1185.69	Joback Method
cpg	1337.06	J/mol×K	1148.16	Joback Method
cpg	1324.07	J/mol×K	1110.64	Joback Method
cpg	1309.66	J/mol×K	1073.12	Joback Method
cpg	1293.76	J/mol×K	1035.60	Joback Method
cpg	1359.03	J/mol×K	1223.21	Joback Method
dvisc	0.0000212	Pa×s	998.08	Joback Method

dvisc	0.0000276	Pa×s	927.66	Joback Method
dvisc	0.0000377	Pa×s	857.24	Joback Method
dvisc	0.0000543	Pa×s	786.82	Joback Method
dvisc	0.0000842	Pa×s	716.39	Joback Method
dvisc	0.0001436	Pa×s	645.97	Joback Method
dvisc	0.0002789	Pa×s	575.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356724&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