Isophthalic acid, pent-4-enyl tridecyl ester

Inchi: InChI=1S/C26H40O4/c1-3-5-7-8-9-10-11-12-13-14-16-21-30-26(28)24-19-17-18-23(22-2
InchiKey: VTYFWYAWCVFBID-UHFFFAOYSA-N
Formula: C26H40O4
SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCC)c1
Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-109.18	kJ/mol	Joback Method
hf	-719.08	kJ/mol	Joback Method
hfus	61.04	kJ/mol	Joback Method
hvap	94.05	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.277		Crippen Method
mcvol	364.020	ml/mol	McGowan Method
pc	938.64	kPa	Joback Method
rinpol	3049.00		NIST Webbook
rinpol	3049.00		NIST Webbook
tb	975.20	K	Joback Method
tc	1194.07	K	Joback Method
tf	564.28	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.85	J/mol×K	975.20	Joback Method
cpg	1230.98	J/mol×K	1011.68	Joback Method
cpg	1246.65	J/mol×K	1048.16	Joback Method
cpg	1260.92	J/mol×K	1084.64	Joback Method
cpg	1273.85	J/mol×K	1121.12	Joback Method
cpg	1285.48	J/mol×K	1157.59	Joback Method
cpg	1295.89	J/mol×K	1194.07	Joback Method
dvisc	0.0003147	Pa×s	564.28	Joback Method

dvisc	0.0001635	Pa×s	632.77	Joback Method
dvisc	0.0000966	Pa×s	701.25	Joback Method
dvisc	0.0000626	Pa×s	769.74	Joback Method
dvisc	0.0000436	Pa×s	838.23	Joback Method
dvisc	0.0000321	Pa×s	906.71	Joback Method
dvisc	0.0000246	Pa×s	975.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356723&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