Isophthalic acid, decyl pent-4-enyl ester

Inchi: InChI=1S/C23H34O4/c1-3-5-7-8-9-10-11-13-18-27-23(25)21-16-14-15-20(19-21)22(24)2
InchiKey: GKLULFBJWJBDDO-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCC)c1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-134.44	kJ/mol	Joback Method
hf	-657.16	kJ/mol	Joback Method
hfus	53.27	kJ/mol	Joback Method
hvap	87.37	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.107		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	2748.00		NIST Webbook
rinpol	2748.00		NIST Webbook
tb	906.56	K	Joback Method
tc	1112.82	K	Joback Method
tf	530.47	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.39	J/mol×K	906.56	Joback Method
cpg	1045.71	J/mol×K	940.94	Joback Method
cpg	1060.79	J/mol×K	975.31	Joback Method
cpg	1074.68	J/mol×K	1009.69	Joback Method
cpg	1087.40	J/mol×K	1044.06	Joback Method
cpg	1098.99	J/mol×K	1078.44	Joback Method
cpg	1109.50	J/mol×K	1112.82	Joback Method
dvisc	0.0004436	Pa×s	530.47	Joback Method

dvisc	0.0002378	Pa×s	593.15	Joback Method
dvisc	0.0001436	Pa×s	655.83	Joback Method
dvisc	0.0000947	Pa×s	718.52	Joback Method
dvisc	0.0000668	Pa×s	781.20	Joback Method
dvisc	0.0000496	Pa×s	843.88	Joback Method
dvisc	0.0000384	Pa×s	906.56	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=U356720&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