Isophthalic acid, dec-2-yl heptyl ester

Inchi: InChI=1S/C25H40O4/c1-4-6-8-10-11-13-16-21(3)29-25(27)23-18-15-17-22(20-23)24(26)
InchiKey: KQBAAKXZSCGZJE-UHFFFAOYSA-N
Formula: C25H40O4
SMILES: CCCCCCCCC(C)OC(=O)c1cccc(C(=O)OCCCCCCC)c1
Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-207.88	kJ/mol	Joback Method
hf	-829.15	kJ/mol	Joback Method
hfus	56.21	kJ/mol	Joback Method
hvap	92.11	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.110		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	975.34	kPa	Joback Method
rinpol	2829.00		NIST Webbook
rinpol	2829.00		NIST Webbook
tb	955.20	K	Joback Method
tc	1169.50	K	Joback Method
tf	539.77	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.72	J/mol×K	955.20	Joback Method
cpg	1198.96	J/mol×K	990.92	Joback Method
cpg	1214.75	J/mol×K	1026.63	Joback Method
cpg	1229.11	J/mol×K	1062.35	Joback Method
cpg	1242.11	J/mol×K	1098.07	Joback Method
cpg	1253.77	J/mol×K	1133.79	Joback Method
cpg	1264.15	J/mol×K	1169.50	Joback Method
dvisc	0.0003804	Pa×s	539.77	Joback Method

dvisc	0.0001851	Pa×s	609.01	Joback Method
dvisc	0.0001043	Pa×s	678.25	Joback Method
dvisc	0.0000654	Pa×s	747.48	Joback Method
dvisc	0.0000443	Pa×s	816.72	Joback Method
dvisc	0.0000320	Pa×s	885.96	Joback Method
dvisc	0.0000242	Pa×s	955.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356511&Units=SI

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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