Isophthalic acid, 3,7-dimethyloct-6-enyl heptyl ester

Inchi: InChI=1S/C25H38O4/c1-5-6-7-8-9-17-28-24(26)22-14-11-15-23(19-22)25(27)29-18-16-2
InchiKey: YBCPWKXANQRJIE-UHFFFAOYSA-N
Formula: C25H38O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)CCC=C(C)C)c1
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-136.21	kJ/mol	Joback Method
hf	-721.72	kJ/mol	Joback Method
hfus	55.10	kJ/mol	Joback Method
hvap	92.14	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	6.743		Crippen Method
mcvol	349.930	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
rinpol	2884.00		NIST Webbook
rinpol	2884.00		NIST Webbook
tb	959.24	K	Joback Method
tc	1175.29	K	Joback Method
tf	520.73	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.18	J/mol×K	959.24	Joback Method
cpg	1170.12	J/mol×K	995.25	Joback Method
cpg	1185.75	J/mol×K	1031.26	Joback Method
cpg	1200.11	J/mol×K	1067.26	Joback Method
cpg	1213.26	J/mol×K	1103.27	Joback Method
cpg	1225.27	J/mol×K	1139.28	Joback Method
cpg	1236.19	J/mol×K	1175.29	Joback Method

Sources

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=U356741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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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