

Isophthalic acid, isoheptyl undec-2-en-1-yl ester

Inchi:	InChI=1S/C25H38O4/c1-4-5-6-7-8-9-10-11-12-18-28-24(26)22-16-13-17-23(20-22)25(27)
InchiKey:	MRKHPAKVJPSULG-VAWYXSNFSA-N
Formula:	C25H38O4
SMILES:	CCCCCCCC=CCOC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]:	402.57

Physical Properties

Property code	Value	Unit	Source
gf	-127.66	kJ/mol	Joback Method
hf	-711.93	kJ/mol	Joback Method
hfus	56.41	kJ/mol	Joback Method
hvap	92.06	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	6.743		Crippen Method
mvol	349.930	ml/mol	McGowan Method
pc	1007.81	kPa	Joback Method
rinpol	3005.00		NIST Webbook
rinpol	3005.00		NIST Webbook
tb	959.36	K	Joback Method
tc	1175.05	K	Joback Method
tf	534.69	K	Joback Method
vc	1.349	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.53	J/molxK	959.36	Joback Method
cpg	1170.43	J/molxK	995.31	Joback Method
cpg	1185.99	J/molxK	1031.26	Joback Method
cpg	1200.29	J/molxK	1067.21	Joback Method
cpg	1213.38	J/molxK	1103.15	Joback Method
cpg	1225.32	J/molxK	1139.10	Joback Method
cpg	1236.16	J/molxK	1175.05	Joback Method
dvisc	0.0003528	Paxs	534.69	Joback Method

dvisc	0.0001679	Paxs	605.47	Joback Method
dvisc	0.0000933	Paxs	676.25	Joback Method
dvisc	0.0000580	Paxs	747.02	Joback Method
dvisc	0.0000391	Paxs	817.80	Joback Method
dvisc	0.0000281	Paxs	888.58	Joback Method
dvisc	0.0000212	Paxs	959.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U343907&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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