

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

Inchi: InChI=1S/C25H38O4/c1-3-5-7-9-10-11-12-13-15-20-29-25(27)23-18-16-17-22(21-23)24(25)
InchiKey: TWRFMHWKIIECRB-FYWRMAATSA-N
Formula: C25H38O4
SMILES: CCCCCCCC=CCOC(=O)c1cccc(C(=O)OCCCCC)c1
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-706.65	kJ/mol	Joback Method
hfus	59.93	kJ/mol	Joback Method
hvap	92.45	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.887		Crippen Method
mvol	349.930	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinpol	3059.00		NIST Webbook
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tb	959.80	K	Joback Method
tc	1175.26	K	Joback Method
tf	549.69	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.14	J/molxK	959.80	Joback Method
cpg	1170.06	J/molxK	995.71	Joback Method
cpg	1185.67	J/molxK	1031.62	Joback Method
cpg	1200.03	J/molxK	1067.53	Joback Method
cpg	1213.20	J/molxK	1103.44	Joback Method
cpg	1225.23	J/molxK	1139.35	Joback Method
cpg	1236.18	J/molxK	1175.26	Joback Method
dvisc	0.0003167	Paxs	549.69	Joback Method

dvisc	0.0001611	Paxs	618.04	Joback Method
dvisc	0.0000938	Paxs	686.39	Joback Method
dvisc	0.0000602	Paxs	754.74	Joback Method
dvisc	0.0000416	Paxs	823.10	Joback Method
dvisc	0.0000304	Paxs	891.45	Joback Method
dvisc	0.0000233	Paxs	959.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343908&Units=SI
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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