

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

Inchi: InChI=1S/C26H40O4/c1-3-5-7-9-10-11-12-14-16-21-30-26(28)24-19-17-18-23(22-24)25(26)
InchiKey: IALKLWFLSRIWPU-JQIJEIRASA-N
Formula: C26H40O4
SMILES: CCCCCCCC=CCOC(=O)c1cccc(C(=O)OCCCCCCC)c1
Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-116.80	kJ/mol	Joback Method
hf	-727.29	kJ/mol	Joback Method
hfus	62.52	kJ/mol	Joback Method
hvap	94.68	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.277		Crippen Method
mvol	364.020	ml/mol	McGowan Method
pc	944.42	kPa	Joback Method
rinpol	3161.00		NIST Webbook
rinpol	3161.00		NIST Webbook
tb	982.68	K	Joback Method
tc	1203.15	K	Joback Method
tf	560.96	K	Joback Method
vc	1.411	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.28	J/molxK	982.68	Joback Method
cpg	1232.52	J/molxK	1019.43	Joback Method
cpg	1248.39	J/molxK	1056.17	Joback Method
cpg	1262.94	J/molxK	1092.92	Joback Method
cpg	1276.23	J/molxK	1129.66	Joback Method
cpg	1288.35	J/molxK	1166.41	Joback Method
cpg	1299.34	J/molxK	1203.15	Joback Method
dvisc	0.0002809	Paxs	560.96	Joback Method

dvisc	0.0001416	Paxs	631.25	Joback Method
dvisc	0.0000818	Paxs	701.53	Joback Method
dvisc	0.0000523	Paxs	771.82	Joback Method
dvisc	0.0000360	Paxs	842.11	Joback Method
dvisc	0.0000262	Paxs	912.39	Joback Method
dvisc	0.0000200	Paxs	982.68	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=U343909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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