

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

Inchi:	InChI=1S/C23H34O4/c1-4-5-6-7-8-9-10-11-12-16-26-22(24)20-14-13-15-21(17-20)23(25)
InchiKey:	MUNZIXKMPXSOOV-VAWYXSNFSA-N
Formula:	C23H34O4
SMILES:	CCCCCCCCC=CCOC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]:	374.51

Physical Properties

Property code	Value	Unit	Source
gf	-144.50	kJ/mol	Joback Method
hf	-670.65	kJ/mol	Joback Method
hfus	51.23	kJ/mol	Joback Method
hvap	87.61	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.963		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1142.89	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	913.60	K	Joback Method
tc	1122.95	K	Joback Method
tf	512.15	K	Joback Method
vc	1.238	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.92	J/molxK	913.60	Joback Method
cpg	1047.33	J/molxK	948.49	Joback Method
cpg	1062.53	J/molxK	983.38	Joback Method
cpg	1076.55	J/molxK	1018.28	Joback Method
cpg	1089.45	J/molxK	1053.17	Joback Method
cpg	1101.27	J/molxK	1088.06	Joback Method
cpg	1112.05	J/molxK	1122.95	Joback Method
dvisc	0.0004475	Paxs	512.15	Joback Method

dvisc	0.0002170	Paxs	579.06	Joback Method
dvisc	0.0001222	Paxs	645.97	Joback Method
dvisc	0.0000767	Paxs	712.88	Joback Method
dvisc	0.0000521	Paxs	779.78	Joback Method
dvisc	0.0000376	Paxs	846.69	Joback Method
dvisc	0.0000285	Paxs	913.60	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=U343904&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
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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