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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002170	Pa×s	579.06	Joback Method
dvisc	0.0001222	Pa×s	645.97	Joback Method
dvisc	0.0000767	Pa×s	712.88	Joback Method
dvisc	0.0000521	Pa×s	779.78	Joback Method
dvisc	0.0000376	Pa×s	846.69	Joback Method
dvisc	0.0000285	Pa×s	913.60	Joback Method

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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