Isophthalic acid, decyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C23H34O4/c1-4-5-6-7-8-9-10-11-16-26-22(24)20-13-12-14-21(18-20)23(25)27
InchiKey: LTRWLFNNKLTDKN-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCC=C(C)C)c1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-150.61	kJ/mol	Joback Method
hf	-675.16	kJ/mol	Joback Method
hfus	53.44	kJ/mol	Joback Method
hvap	88.08	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.107		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2854.00		NIST Webbook
rinpol	2854.00		NIST Webbook
tb	913.92	K	Joback Method
tc	1123.15	K	Joback Method
tf	513.19	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.09	J/mol×K	913.92	Joback Method
cpg	1046.54	J/mol×K	948.79	Joback Method
cpg	1061.79	J/mol×K	983.66	Joback Method
cpg	1075.89	J/mol×K	1018.53	Joback Method
cpg	1088.89	J/mol×K	1053.40	Joback Method
cpg	1100.83	J/mol×K	1088.27	Joback Method
cpg	1111.75	J/mol×K	1123.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343942&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
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