Isophthalic acid, decyl 3-methylbutyl ester

Inchi: InChI=1S/C23H36O4/c1-4-5-6-7-8-9-10-11-16-26-22(24)20-13-12-14-21(18-20)23(25)27
InchiKey: NYMFSTKWRADONF-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)c1
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-224.72	kJ/mol	Joback Method
hf	-787.87	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.187		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	2717.00		NIST Webbook
tb	909.44	K	Joback Method
tc	1116.16	K	Joback Method
tf	517.23	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.53	J/mol×K	909.44	Joback Method
cpg	1075.35	J/mol×K	943.89	Joback Method
cpg	1090.85	J/mol×K	978.35	Joback Method
cpg	1105.07	J/mol×K	1012.80	Joback Method
cpg	1118.04	J/mol×K	1047.26	Joback Method
cpg	1129.80	J/mol×K	1081.71	Joback Method
cpg	1140.38	J/mol×K	1116.16	Joback Method
dvisc	0.0004827	Pa×s	517.23	Joback Method
dvisc	0.0002394	Pa×s	582.60	Joback Method

dvisc	0.0001368	Pa×s	647.97	Joback Method
dvisc	0.0000866	Pa×s	713.34	Joback Method
dvisc	0.0000592	Pa×s	778.70	Joback Method
dvisc	0.0000429	Pa×s	844.07	Joback Method
dvisc	0.0000326	Pa×s	909.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356465&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/68-134-8/Isophthalic-acid-decyl-3-methylbutyl-ester.pdf
Generated by Cheméo on 2024-10-12 09:11:46.206019509 +0000 UTC m=+3305168.842988757.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.