Isophthalic acid, monoamide, N,N-diisobutyl-, octyl ester

Other names: Isophthalic acid, monoamide, N-diisobutyl-, octyl ester
Inchi: InChI=1S/C24H39NO3/c1-6-7-8-9-10-11-15-28-24(27)22-14-12-13-21(16-22)23(26)25(17
InchiKey: XFCNBVHJZLKUCP-UHFFFAOYSA-N
Formula: C24H39NO3
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]: 389.57

Physical Properties

Property code	Value	Unit	Source
gf	-2.96	kJ/mol	Joback Method
hf	-614.04	kJ/mol	Joback Method
hfus	51.93	kJ/mol	Joback Method
hvap	89.12	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.958		Crippen Method
mcvol	344.250	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2838.00		NIST Webbook
rinpol	2838.00		NIST Webbook
tb	921.90	K	Joback Method
tc	1130.66	K	Joback Method
tf	523.74	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.71	J/mol×K	921.90	Joback Method
cpg	1151.38	J/mol×K	956.69	Joback Method
cpg	1167.77	J/mol×K	991.49	Joback Method
cpg	1182.93	J/mol×K	1026.28	Joback Method
cpg	1196.92	J/mol×K	1061.08	Joback Method
cpg	1209.80	J/mol×K	1095.87	Joback Method
cpg	1221.64	J/mol×K	1130.66	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=U345801&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
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