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

Other names: Isophthalic acid, monoamide, N-diisobutyl-, undecyl ester
Inchi: InChI=1S/C27H45NO3/c1-6-7-8-9-10-11-12-13-14-18-31-27(30)25-17-15-16-24(19-25)26
InchiKey: PCCHTTQOJLEPNS-UHFFFAOYSA-N
Formula: C27H45NO3
SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]: 431.65

Physical Properties

Property code	Value	Unit	Source
gf	22.30	kJ/mol	Joback Method
hf	-675.96	kJ/mol	Joback Method
hfus	59.70	kJ/mol	Joback Method
hvap	95.80	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	7.128		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	3160.00		NIST Webbook
rinpol	3160.00		NIST Webbook
tb	990.54	K	Joback Method
tc	1213.22	K	Joback Method
tf	557.55	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.49	J/mol×K	990.54	Joback Method
cpg	1340.05	J/mol×K	1027.65	Joback Method
cpg	1357.14	J/mol×K	1064.77	Joback Method
cpg	1372.84	J/mol×K	1101.88	Joback Method
cpg	1387.24	J/mol×K	1138.99	Joback Method
cpg	1400.42	J/mol×K	1176.11	Joback Method
cpg	1412.46	J/mol×K	1213.22	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=U345804&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