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

Other names: Isophthalic acid, monoamide, N-diisobutyl-, nonyl ester
Inchi: InChI=1S/C25H41NO3/c1-6-7-8-9-10-11-12-16-29-25(28)23-15-13-14-22(17-23)24(27)26
InchiKey: SMBNKDQUBPNXLW-UHFFFAOYSA-N
Formula: C25H41NO3
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]: 403.60

Physical Properties

Property code	Value	Unit	Source
gf	5.46	kJ/mol	Joback Method
hf	-634.68	kJ/mol	Joback Method
hfus	54.52	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.348		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	2941.00		NIST Webbook
rinpol	2941.00		NIST Webbook
tb	944.78	K	Joback Method
tc	1157.19	K	Joback Method
tf	535.01	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.80	J/mol×K	944.78	Joback Method
cpg	1213.73	J/mol×K	980.18	Joback Method
cpg	1230.32	J/mol×K	1015.58	Joback Method
cpg	1245.64	J/mol×K	1050.99	Joback Method
cpg	1259.75	J/mol×K	1086.39	Joback Method
cpg	1272.72	J/mol×K	1121.79	Joback Method
cpg	1284.62	J/mol×K	1157.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345802&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