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

Other names: Isophthalic acid, monoamide, N-diisobutyl-, propyl ester
Inchi: InChI=1S/C19H29NO3/c1-6-10-23-19(22)17-9-7-8-16(11-17)18(21)20(12-14(2)3)13-15(4
InchiKey: GQLKZOGWGVSPBI-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: CCCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	-45.06	kJ/mol	Joback Method
hf	-510.84	kJ/mol	Joback Method
hfus	38.98	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.008		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2318.00		NIST Webbook
tb	807.50	K	Joback Method
tc	1010.32	K	Joback Method
tf	467.39	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.78	J/mol×K	807.50	Joback Method
cpg	849.50	J/mol×K	841.30	Joback Method
cpg	865.10	J/mol×K	875.11	Joback Method
cpg	879.61	J/mol×K	908.91	Joback Method
cpg	893.08	J/mol×K	942.71	Joback Method
cpg	905.54	J/mol×K	976.52	Joback Method
cpg	917.05	J/mol×K	1010.32	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=U345795&Units=SI

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