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

Other names: Isophthalic acid, monoamide, N-diisobutyl-, isobutyl ester
Inchi: InChI=1S/C20H31NO3/c1-14(2)11-21(12-15(3)4)19(22)17-8-7-9-18(10-17)20(23)24-13-1
InchiKey: UVRWKWAQTWYTRE-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CC(C)COC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
gf	-39.08	kJ/mol	Joback Method
hf	-536.76	kJ/mol	Joback Method
hfus	38.05	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.254		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	829.94	K	Joback Method
tc	1034.59	K	Joback Method
tf	463.66	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.02	J/mol×K	829.94	Joback Method
cpg	909.08	J/mol×K	864.05	Joback Method
cpg	924.95	J/mol×K	898.16	Joback Method
cpg	939.69	J/mol×K	932.27	Joback Method
cpg	953.34	J/mol×K	966.38	Joback Method
cpg	965.93	J/mol×K	1000.48	Joback Method
cpg	977.53	J/mol×K	1034.59	Joback Method

Sources

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=U345796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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