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

Other names: Isophthalic acid, monoamide, N-diisobutyl-, dodecyl ester
Inchi: InChI=1S/C28H47NO3/c1-6-7-8-9-10-11-12-13-14-15-19-32-28(31)26-18-16-17-25(20-26
InchiKey: POGWAMWGVUNNDD-UHFFFAOYSA-N
Formula: C28H47NO3
SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]: 445.68

Physical Properties

Property code	Value	Unit	Source
gf	30.72	kJ/mol	Joback Method
hf	-696.60	kJ/mol	Joback Method
hfus	62.29	kJ/mol	Joback Method
hvap	98.03	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	7.518		Crippen Method
mcvol	400.610	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3254.00		NIST Webbook
rinpol	3254.00		NIST Webbook
tb	1013.42	K	Joback Method
tc	1242.86	K	Joback Method
tf	568.82	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.99	J/mol×K	1013.42	Joback Method
cpg	1403.94	J/mol×K	1051.66	Joback Method
cpg	1421.34	J/mol×K	1089.90	Joback Method
cpg	1437.28	J/mol×K	1128.14	Joback Method
cpg	1451.85	J/mol×K	1166.38	Joback Method
cpg	1465.16	J/mol×K	1204.62	Joback Method
cpg	1477.30	J/mol×K	1242.86	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=U345805&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