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

Other names: Isophthalic acid, monoamide, N-diisobutyl-, decyl ester
Inchi: InChI=1S/C26H43NO3/c1-6-7-8-9-10-11-12-13-17-30-26(29)24-16-14-15-23(18-24)25(28
InchiKey: DMJGYSRWVQBNIE-UHFFFAOYSA-N
Formula: C26H43NO3
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]: 417.62

Physical Properties

Property code	Value	Unit	Source
gf	13.88	kJ/mol	Joback Method
hf	-655.32	kJ/mol	Joback Method
hfus	57.11	kJ/mol	Joback Method
hvap	93.58	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	6.738		Crippen Method
mcvol	372.430	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		NIST Webbook
tb	967.66	K	Joback Method
tc	1184.69	K	Joback Method
tf	546.28	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.41	J/mol×K	967.66	Joback Method
cpg	1276.63	J/mol×K	1003.83	Joback Method
cpg	1293.46	J/mol×K	1040.00	Joback Method
cpg	1308.95	J/mol×K	1076.17	Joback Method
cpg	1323.20	J/mol×K	1112.34	Joback Method
cpg	1336.27	J/mol×K	1148.52	Joback Method
cpg	1348.23	J/mol×K	1184.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345803&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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