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

Inchi: InChI=1S/C26H43NO3/c1-5-7-9-11-13-18-27(19-14-12-10-8-6-2)25(28)23-16-15-17-24(2

InchiKey: QPFSHALLEYQUPX-UHFFFAOYSA-N

Formula: C26H43NO3

SMILES: CCCCCCCN(CCCCCCC)C(=O)c1cccc(C(=O)OCC(C)C)c1

Mol. weight [g/mol]: 417.62

Physical Properties

Property code	Value	Unit	Source
gf	16.32	kJ/mol	Joback Method
hf	-650.04	kJ/mol	Joback Method
hfus	60.63	kJ/mol	Joback Method
hvap	93.97	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	6.882		Crippen Method
mcvol	372.430	ml/mol	McGowan Method
pc	927.81	kPa	Joback Method
rinpol	3048.00		NIST Webbook
rinpol	3048.00		NIST Webbook
tb	968.10	K	Joback Method
tc	1185.30	K	Joback Method
tf	561.28	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.04	J/mol×K	968.10	Joback Method
cpg	1276.33	J/mol×K	1004.30	Joback Method
cpg	1293.23	J/mol×K	1040.50	Joback Method
cpg	1308.81	J/mol×K	1076.70	Joback Method
cpg	1323.15	J/mol×K	1112.90	Joback Method
cpg	1336.33	J/mol×K	1149.10	Joback Method
cpg	1348.42	J/mol×K	1185.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345825&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