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

Inchi: InChI=1S/C27H45NO3/c1-4-7-10-12-14-20-28(21-15-13-11-8-5-2)26(29)24-18-17-19-25(

InchiKey: HHDDJKAPAQVUKJ-UHFFFAOYSA-N

Formula: C27H45NO3

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

Mol. weight [g/mol]: 431.65

Physical Properties

Property code	Value	Unit	Source
gf	27.18	kJ/mol	Joback Method
hf	-665.40	kJ/mol	Joback Method
hfus	66.75	kJ/mol	Joback Method
hvap	96.58	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.417		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	871.71	kPa	Joback Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook
tb	991.42	K	Joback Method
tc	1215.43	K	Joback Method
tf	587.55	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.83	J/mol×K	991.42	Joback Method
cpg	1339.62	J/mol×K	1028.75	Joback Method
cpg	1356.95	J/mol×K	1066.09	Joback Method
cpg	1372.90	J/mol×K	1103.42	Joback Method
cpg	1387.57	J/mol×K	1140.76	Joback Method
cpg	1401.03	J/mol×K	1178.09	Joback Method
cpg	1413.37	J/mol×K	1215.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345827&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