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

Inchi: InChI=1S/C28H47NO3/c1-4-7-10-13-15-21-29(22-16-14-11-8-5-2)27(30)25-19-18-20-26(

InchiKey: KJRWJJOSYNCZHS-UHFFFAOYSA-N

Formula: C28H47NO3

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

Mol. weight [g/mol]: 445.68

Physical Properties

Property code	Value	Unit	Source
gf	35.60	kJ/mol	Joback Method
hf	-686.04	kJ/mol	Joback Method
hfus	69.34	kJ/mol	Joback Method
hvap	98.80	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	7.807		Crippen Method
mcvol	400.610	ml/mol	McGowan Method
pc	824.31	kPa	Joback Method
rinpol	3296.00		NIST Webbook
rinpol	3296.00		NIST Webbook
tb	1014.30	K	Joback Method
tc	1245.94	K	Joback Method
tf	598.82	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.43	J/mol×K	1014.30	Joback Method
cpg	1403.69	J/mol×K	1052.91	Joback Method
cpg	1421.41	J/mol×K	1091.51	Joback Method
cpg	1437.66	J/mol×K	1130.12	Joback Method
cpg	1452.57	J/mol×K	1168.73	Joback Method
cpg	1466.22	J/mol×K	1207.34	Joback Method
cpg	1478.71	J/mol×K	1245.94	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=U345829&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