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

Inchi: InChI=1S/C28H47NO3/c1-5-7-9-11-13-20-29(21-14-12-10-8-6-2)27(30)25-18-15-19-26(2

InchiKey: JJNOIXCRFMIBTA-UHFFFAOYSA-N

Formula: C28H47NO3

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

Mol. weight [g/mol]: 445.68

Physical Properties

Property code	Value	Unit	Source
gf	33.16	kJ/mol	Joback Method
hf	-691.32	kJ/mol	Joback Method
hfus	65.81	kJ/mol	Joback Method
hvap	98.42	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	7.663		Crippen Method
mcvol	400.610	ml/mol	McGowan Method
pc	828.11	kPa	Joback Method
rinpol	3248.00		NIST Webbook
rinpol	3248.00		NIST Webbook
tb	1013.86	K	Joback Method
tc	1244.32	K	Joback Method
tf	583.82	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.71	J/mol×K	1013.86	Joback Method
cpg	1403.81	J/mol×K	1052.27	Joback Method
cpg	1421.36	J/mol×K	1090.68	Joback Method
cpg	1437.45	J/mol×K	1129.09	Joback Method
cpg	1452.19	J/mol×K	1167.50	Joback Method
cpg	1465.66	J/mol×K	1205.91	Joback Method
cpg	1477.98	J/mol×K	1244.32	Joback Method

Sources

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=U345828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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