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

Inchi: InChI=1S/C31H53NO3/c1-4-7-10-13-14-17-20-26-35-31(34)29-23-21-22-28(27-29)30(33

InchiKey: BSODHWJZYYQAPX-UHFFFAOYSA-N

Formula: C31H53NO3

SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)N(CCCCCCC)CCCCCCC)c1

Mol. weight [g/mol]: 487.76

Physical Properties

Property code	Value	Unit	Source
gf	60.86	kJ/mol	Joback Method
hf	-747.96	kJ/mol	Joback Method
hfus	77.11	kJ/mol	Joback Method
hvap	105.48	kJ/mol	Joback Method
log10ws	-10.23		Crippen Method
logp	8.977		Crippen Method
mcvol	442.880	ml/mol	McGowan Method
pc	703.21	kPa	Joback Method
rinpol	3612.00		NIST Webbook
rinpol	3612.00		NIST Webbook
tb	1082.94	K	Joback Method
tc	1345.36	K	Joback Method
tf	632.63	K	Joback Method
vc	1.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1577.46	J/mol×K	1082.94	Joback Method
cpg	1598.54	J/mol×K	1126.68	Joback Method
cpg	1617.71	J/mol×K	1170.41	Joback Method
cpg	1635.13	J/mol×K	1214.15	Joback Method
cpg	1650.96	J/mol×K	1257.88	Joback Method
cpg	1665.36	J/mol×K	1301.62	Joback Method
cpg	1678.50	J/mol×K	1345.36	Joback Method

Sources

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=U345832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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