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

Inchi: InChI=1S/C30H51NO3/c1-4-7-10-13-16-19-25-34-30(33)28-22-20-21-27(26-28)29(32)31

InchiKey: XXTXTEFGHDHPDP-UHFFFAOYSA-N

Formula: C30H51NO3

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

Mol. weight [g/mol]: 473.73

Physical Properties

Property code	Value	Unit	Source
gf	52.44	kJ/mol	Joback Method
hf	-727.32	kJ/mol	Joback Method
hfus	74.51	kJ/mol	Joback Method
hvap	103.26	kJ/mol	Joback Method
log10ws	-9.81		Crippen Method
logp	8.587		Crippen Method
mcvol	428.790	ml/mol	McGowan Method
pc	740.43	kPa	Joback Method
rinpol	3492.00		NIST Webbook
rinpol	3492.00		NIST Webbook
tb	1060.06	K	Joback Method
tc	1310.81	K	Joback Method
tf	621.36	K	Joback Method
vc	1.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1512.77	J/mol×K	1060.06	Joback Method
cpg	1533.18	J/mol×K	1101.85	Joback Method
cpg	1551.81	J/mol×K	1143.64	Joback Method
cpg	1568.79	J/mol×K	1185.43	Joback Method
cpg	1584.28	J/mol×K	1227.23	Joback Method
cpg	1598.39	J/mol×K	1269.02	Joback Method
cpg	1611.27	J/mol×K	1310.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345831&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

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