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

Inchi: InChI=1S/C29H49NO3/c1-4-7-10-13-16-22-30(23-17-14-11-8-5-2)28(31)26-20-19-21-27(

InchiKey: OPIDBDJHDLVIFW-UHFFFAOYSA-N

Formula: C29H49NO3

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

Mol. weight [g/mol]: 459.70

Physical Properties

Property code	Value	Unit	Source
gf	44.02	kJ/mol	Joback Method
hf	-706.68	kJ/mol	Joback Method
hfus	71.92	kJ/mol	Joback Method
hvap	101.03	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.197		Crippen Method
mcvol	414.700	ml/mol	McGowan Method
pc	780.69	kPa	Joback Method
rinpol	3396.00		NIST Webbook
rinpol	3396.00		NIST Webbook
tb	1037.18	K	Joback Method
tc	1277.71	K	Joback Method
tf	610.09	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1448.42	J/mol×K	1037.18	Joback Method
cpg	1468.22	J/mol×K	1077.27	Joback Method
cpg	1486.37	J/mol×K	1117.36	Joback Method
cpg	1502.97	J/mol×K	1157.44	Joback Method
cpg	1518.15	J/mol×K	1197.53	Joback Method
cpg	1532.01	J/mol×K	1237.62	Joback Method
cpg	1544.68	J/mol×K	1277.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345830&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