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

Inchi: InChI=1S/C24H39NO3/c1-4-7-9-11-13-18-25(19-14-12-10-8-5-2)23(26)21-16-15-17-22(2

InchiKey: XKSBGGZZLQNYSN-UHFFFAOYSA-N

Formula: C24H39NO3

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

Mol. weight [g/mol]: 389.57

Physical Properties

Property code	Value	Unit	Source
gf	1.92	kJ/mol	Joback Method
hf	-603.48	kJ/mol	Joback Method
hfus	58.98	kJ/mol	Joback Method
hvap	89.90	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	6.246		Crippen Method
mcvol	344.250	ml/mol	McGowan Method
pc	1041.25	kPa	Joback Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook
tb	922.78	K	Joback Method
tc	1130.50	K	Joback Method
tf	553.74	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.85	J/mol×K	922.78	Joback Method
cpg	1150.50	J/mol×K	957.40	Joback Method
cpg	1166.90	J/mol×K	992.02	Joback Method
cpg	1182.11	J/mol×K	1026.64	Joback Method
cpg	1196.19	J/mol×K	1061.26	Joback Method
cpg	1209.20	J/mol×K	1095.88	Joback Method
cpg	1221.19	J/mol×K	1130.50	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=U345823&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

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