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

Inchi: InChI=1S/C26H43NO3/c1-4-7-10-12-14-19-27(20-15-13-11-8-5-2)25(28)23-17-16-18-24(

InchiKey: FQXPEGJUOXCWJB-UHFFFAOYSA-N

Formula: C26H43NO3

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

Mol. weight [g/mol]: 417.62

Physical Properties

Property code	Value	Unit	Source
gf	18.76	kJ/mol	Joback Method
hf	-644.76	kJ/mol	Joback Method
hfus	64.16	kJ/mol	Joback Method
hvap	94.35	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.026		Crippen Method
mcvol	372.430	ml/mol	McGowan Method
pc	923.30	kPa	Joback Method
rinpol	3101.00		NIST Webbook
rinpol	3101.00		NIST Webbook
tb	968.54	K	Joback Method
tc	1186.07	K	Joback Method
tf	576.28	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.68	J/mol×K	968.54	Joback Method
cpg	1276.04	J/mol×K	1004.79	Joback Method
cpg	1293.03	J/mol×K	1041.05	Joback Method
cpg	1308.70	J/mol×K	1077.30	Joback Method
cpg	1323.15	J/mol×K	1113.56	Joback Method
cpg	1336.44	J/mol×K	1149.81	Joback Method
cpg	1348.66	J/mol×K	1186.07	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=U345826&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

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