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

Inchi: InChI=1S/C25H41NO3/c1-4-7-9-11-13-18-26(19-14-12-10-8-5-2)24(27)22-16-15-17-23(2

InchiKey: MEYFTLOWWJJBQK-UHFFFAOYSA-N

Formula: C25H41NO3

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

Mol. weight [g/mol]: 403.60

Physical Properties

Property code	Value	Unit	Source
gf	10.34	kJ/mol	Joback Method
hf	-624.12	kJ/mol	Joback Method
hfus	61.56	kJ/mol	Joback Method
hvap	92.13	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	6.636		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	979.62	kPa	Joback Method
rinpol	3002.00		NIST Webbook
rinpol	3002.00		NIST Webbook
tb	945.66	K	Joback Method
tc	1157.78	K	Joback Method
tf	565.01	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.00	J/mol×K	945.66	Joback Method
cpg	1212.99	J/mol×K	981.01	Joback Method
cpg	1229.67	J/mol×K	1016.37	Joback Method
cpg	1245.10	J/mol×K	1051.72	Joback Method
cpg	1259.35	J/mol×K	1087.07	Joback Method
cpg	1272.49	J/mol×K	1122.43	Joback Method
cpg	1284.59	J/mol×K	1157.78	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345824&Units=SI

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