

Pimelic acid, hexyl 4-nitrophenyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H27NO6/c1-2-3-4-8-15-25-18(21)9-6-5-7-10-19(22)26-17-13-11-16(12-14-

GOEOQQPUWXLWJW-UHFFFAOYSA-N

C19H27NO6

CCCCCOC(=O)CCCCC(=O)Oc1ccc([N+](=O)[O-])cc1

365.42

Physical Properties

Property code	Value	Unit	Source
gf	-220.41	kJ/mol	Joback Method
hf	-710.79	kJ/mol	Joback Method
hfus	55.55	kJ/mol	Joback Method
hvap	95.73	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.574		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2897.00		NIST Webbook
tb	970.20	K	Joback Method
tc	1193.92	K	Joback Method
tf	630.76	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.17	J/mol×K	970.20	Joback Method
cpg	941.66	J/mol×K	1007.49	Joback Method
cpg	952.85	J/mol×K	1044.77	Joback Method
cpg	962.77	J/mol×K	1082.06	Joback Method
cpg	971.45	J/mol×K	1119.34	Joback Method
cpg	978.94	J/mol×K	1156.63	Joback Method
cpg	985.26	J/mol×K	1193.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416620&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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