

Pimelic acid, 3-nitrophenyl propyl ester

Inchi:	InChI=1S/C16H21NO6/c1-2-11-22-15(18)9-4-3-5-10-16(19)23-14-8-6-7-13(12-14)17(20)
InchiKey:	WFFZLCAVLMLOPK-UHFFFAOYSA-N
Formula:	C16H21NO6
SMILES:	CCCOC(=O)CCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	323.34

Physical Properties

Property code	Value	Unit	Source
gf	-245.67	kJ/mol	Joback Method
hf	-648.87	kJ/mol	Joback Method
hfus	47.78	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.404		Crippen Method
mvol	244.840	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook
tb	901.56	K	Joback Method
tc	1124.04	K	Joback Method
tf	596.95	K	Joback Method
vc	0.954	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.95	J/molxK	901.56	Joback Method
cpg	767.04	J/molxK	938.64	Joback Method
cpg	777.96	J/molxK	975.72	Joback Method
cpg	787.73	J/molxK	1012.80	Joback Method
cpg	796.37	J/molxK	1049.88	Joback Method
cpg	803.89	J/molxK	1086.96	Joback Method
cpg	810.33	J/molxK	1124.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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