Glutaric acid, hexyl 2-(4-nitrophenoxy)ethyl ester

Inchi: InChI=1S/C19H27NO7/c1-2-3-4-5-13-26-18(21)7-6-8-19(22)27-15-14-25-17-11-9-16(10-
InchiKey: KWUFBWUAWOFLGX-UHFFFAOYSA-N
Formula: C19H27NO7
SMILES: CCCCCCOC(=O)CCCC(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 381.42

Physical Properties

Property code	Value	Unit	Source
gf	-325.41	kJ/mol	Joback Method
hf	-843.01	kJ/mol	Joback Method
hfus	56.74	kJ/mol	Joback Method
hvap	98.14	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.811		Crippen Method
mcvol	292.980	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	3005.00		NIST Webbook
tb	992.62	K	Joback Method
tc	1218.67	K	Joback Method
tf	652.99	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.38	J/mol×K	992.62	Joback Method
cpg	966.94	J/mol×K	1030.29	Joback Method
cpg	977.02	J/mol×K	1067.97	Joback Method
cpg	985.65	J/mol×K	1105.64	Joback Method
cpg	992.84	J/mol×K	1143.32	Joback Method
cpg	998.61	J/mol×K	1180.99	Joback Method
cpg	1002.97	J/mol×K	1218.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376798&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

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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