Glutaric acid, 2-methylhex-3-yl 2-(4-nitrophenoxy)ethyl ester

Inchi: InChI=1S/C20H29NO7/c1-4-6-18(15(2)3)28-20(23)8-5-7-19(22)27-14-13-26-17-11-9-16(

InchiKey: LVZGUAWZFLXNRC-UHFFFAOYSA-N

Formula: C20H29NO7

SMILES: CCCC(OC(=O)CCCC(=O)OCCOc1ccc([N+](=O)[O-])cc1)C(C)C

Mol. weight [g/mol]: 395.45

Physical Properties

Property code	Value	Unit	Source
gf	-321.87	kJ/mol	Joback Method
hf	-874.21	kJ/mol	Joback Method
hfus	52.28	kJ/mol	Joback Method
hvap	99.59	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.055		Crippen Method
mcvol	307.070	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	2963.00		NIST Webbook
tb	1014.62	K	Joback Method
tc	1245.08	K	Joback Method
tf	634.26	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.23	J/mol×K	1014.62	Joback Method
cpg	1026.74	J/mol×K	1053.03	Joback Method
cpg	1036.65	J/mol×K	1091.44	Joback Method
cpg	1044.98	J/mol×K	1129.85	Joback Method
cpg	1051.76	J/mol×K	1168.26	Joback Method
cpg	1057.01	J/mol×K	1206.67	Joback Method
cpg	1060.74	J/mol×K	1245.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376797&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