Glutaric acid, 8-chlorooctyl 3-nitrobenzyl ester

Inchi: InChI=1S/C20H28ClNO6/c21-13-5-3-1-2-4-6-14-27-19(23)11-8-12-20(24)28-16-17-9-7-1
InchiKey: QXPPVBZDXLXHGO-UHFFFAOYSA-N
Formula: C20H28ClNO6
SMILES: O=C(CCCC(=O)OCc1cccc([N+](=O)[O-])c1)OCCCCCCCCCl
Mol. weight [g/mol]: 413.89

Physical Properties

Property code	Value	Unit	Source
gf	-223.92	kJ/mol	Joback Method
hf	-747.17	kJ/mol	Joback Method
hfus	62.34	kJ/mol	Joback Method
hvap	102.34	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.931		Crippen Method
mcvol	313.440	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	3289.00		NIST Webbook
rinpol	3289.00		NIST Webbook
tb	1030.51	K	Joback Method
tc	1263.07	K	Joback Method
tf	671.95	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.03	J/mol×K	1030.51	Joback Method
cpg	1020.35	J/mol×K	1069.27	Joback Method
cpg	1030.30	J/mol×K	1108.03	Joback Method
cpg	1038.93	J/mol×K	1146.79	Joback Method
cpg	1046.28	J/mol×K	1185.55	Joback Method
cpg	1052.40	J/mol×K	1224.31	Joback Method
cpg	1057.32	J/mol×K	1263.07	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=U393363&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

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