Glutaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, nonyl ester

Inchi: InChI=1S/C21H32ClNO4/c1-3-4-5-6-7-8-9-15-27-21(25)12-10-11-20(24)23-18-16-17(22)

InchiKey: IHKKLQJXTJDSLF-UHFFFAOYSA-N

Formula: C21H32ClNO4

SMILES: CCCCCCCCCOC(=O)CCCC(=O)Nc1cc(Cl)ccc1OC

Mol. weight [g/mol]: 397.94

Physical Properties

Property code	Value	Unit	Source
gf	-171.29	kJ/mol	Joback Method
hf	-715.05	kJ/mol	Joback Method
hfus	58.28	kJ/mol	Joback Method
hvap	95.07	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.751		Crippen Method
mcvol	320.090	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	3303.00		NIST Webbook
tb	956.70	K	Joback Method
tc	1172.50	K	Joback Method
tf	604.79	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1021.37	J/mol×K	956.70	Joback Method
cpg	1035.59	J/mol×K	992.67	Joback Method
cpg	1048.50	J/mol×K	1028.63	Joback Method
cpg	1060.12	J/mol×K	1064.60	Joback Method
cpg	1070.48	J/mol×K	1100.57	Joback Method
cpg	1079.61	J/mol×K	1136.53	Joback Method
cpg	1087.55	J/mol×K	1172.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360759&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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