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

Inchi: InChI=1S/C17H24ClNO4/c1-3-4-5-11-23-17(21)8-6-7-16(20)19-14-12-13(18)9-10-15(14)22-2

InchiKey: LGPIFVUFENFBFL-UHFFFAOYSA-N

Formula: C17H24ClNO4

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

Mol. weight [g/mol]: 341.83

Physical Properties

Property code	Value	Unit	Source
gf	-204.97	kJ/mol	Joback Method
hf	-632.49	kJ/mol	Joback Method
hfus	47.92	kJ/mol	Joback Method
hvap	86.17	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.191		Crippen Method
mcvol	263.730	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2897.00		NIST Webbook
tb	865.18	K	Joback Method
tc	1073.69	K	Joback Method
tf	559.71	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.96	J/mol×K	865.18	Joback Method
cpg	799.37	J/mol×K	899.93	Joback Method
cpg	811.69	J/mol×K	934.68	Joback Method
cpg	822.94	J/mol×K	969.43	Joback Method
cpg	833.14	J/mol×K	1004.19	Joback Method
cpg	842.29	J/mol×K	1038.94	Joback Method
cpg	850.42	J/mol×K	1073.69	Joback Method

Sources

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=U360755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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