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

Inchi: InChI=1S/C14H18ClNO4/c1-3-20-14(18)6-4-5-13(17)16-11-9-10(15)7-8-12(11)19-2/h7-9
InchiKey: CDUXWNNQFRINAJ-UHFFFAOYSA-N
Formula: C14H18ClNO4
SMILES: CCOC(=O)CCCC(=O)Nc1cc(Cl)ccc1OC
Mol. weight [g/mol]: 299.75

Physical Properties

Property code	Value	Unit	Source
gf	-230.23	kJ/mol	Joback Method
hf	-570.57	kJ/mol	Joback Method
hfus	40.15	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.021		Crippen Method
mcvol	221.460	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	2601.00		NIST Webbook
tb	796.54	K	Joback Method
tc	1007.40	K	Joback Method
tf	525.90	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.45	J/mol×K	796.54	Joback Method
cpg	630.04	J/mol×K	831.68	Joback Method
cpg	641.68	J/mol×K	866.83	Joback Method
cpg	652.36	J/mol×K	901.97	Joback Method
cpg	662.10	J/mol×K	937.11	Joback Method
cpg	670.90	J/mol×K	972.25	Joback Method
cpg	678.77	J/mol×K	1007.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360751&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