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

Inchi: InChI=1S/C15H20ClNO4/c1-3-9-21-15(19)6-4-5-14(18)17-12-10-11(16)7-8-13(12)20-2/h
InchiKey: PDLAIOBPEYGJHP-UHFFFAOYSA-N
Formula: C15H20ClNO4
SMILES: CCCOC(=O)CCCC(=O)Nc1cc(Cl)ccc1OC
Mol. weight [g/mol]: 313.78

Physical Properties

Property code	Value	Unit	Source
gf	-221.81	kJ/mol	Joback Method
hf	-591.21	kJ/mol	Joback Method
hfus	42.74	kJ/mol	Joback Method
hvap	81.72	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.411		Crippen Method
mcvol	235.550	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	2693.00		NIST Webbook
tb	819.42	K	Joback Method
tc	1028.85	K	Joback Method
tf	537.17	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.71	J/mol×K	819.42	Joback Method
cpg	685.61	J/mol×K	854.32	Joback Method
cpg	697.52	J/mol×K	889.23	Joback Method
cpg	708.43	J/mol×K	924.13	Joback Method
cpg	718.37	J/mol×K	959.04	Joback Method
cpg	727.33	J/mol×K	993.94	Joback Method
cpg	735.33	J/mol×K	1028.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360752&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