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

Inchi: InChI=1S/C22H34ClNO4/c1-3-4-5-6-7-8-9-10-16-28-22(26)13-11-12-21(25)24-19-17-18(
InchiKey: SSSUPUUNJWNTKP-UHFFFAOYSA-N
Formula: C22H34ClNO4
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)Nc1cc(Cl)ccc1OC
Mol. weight [g/mol]: 411.96

Physical Properties

Property code	Value	Unit	Source
gf	-162.87	kJ/mol	Joback Method
hf	-735.69	kJ/mol	Joback Method
hfus	60.87	kJ/mol	Joback Method
hvap	97.30	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.141		Crippen Method
mcvol	334.180	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	3400.00		NIST Webbook
tb	979.58	K	Joback Method
tc	1199.44	K	Joback Method
tf	616.06	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1081.71	J/mol×K	979.58	Joback Method
cpg	1096.13	J/mol×K	1016.22	Joback Method
cpg	1109.17	J/mol×K	1052.87	Joback Method
cpg	1120.84	J/mol×K	1089.51	Joback Method
cpg	1131.18	J/mol×K	1126.15	Joback Method
cpg	1140.24	J/mol×K	1162.80	Joback Method
cpg	1148.03	J/mol×K	1199.44	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=U360760&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