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

Inchi: InChI=1S/C18H26ClNO4/c1-3-4-5-6-12-24-18(22)9-7-8-17(21)20-15-13-14(19)10-11-16(

InchiKey: FQTJYNNSDHXBQX-UHFFFAOYSA-N

Formula: C18H26ClNO4

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

Mol. weight [g/mol]: 355.86

Physical Properties

Property code	Value	Unit	Source
gf	-196.55	kJ/mol	Joback Method
hf	-653.13	kJ/mol	Joback Method
hfus	50.51	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.581		Crippen Method
mcvol	277.820	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	3008.00		NIST Webbook
rinpol	3008.00		NIST Webbook
tb	888.06	K	Joback Method
tc	1097.17	K	Joback Method
tf	570.98	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.80	J/mol×K	888.06	Joback Method
cpg	857.42	J/mol×K	922.91	Joback Method
cpg	869.91	J/mol×K	957.76	Joback Method
cpg	881.29	J/mol×K	992.61	Joback Method
cpg	891.57	J/mol×K	1027.47	Joback Method
cpg	900.76	J/mol×K	1062.32	Joback Method
cpg	908.89	J/mol×K	1097.17	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=U360757&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