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

Inchi: InChI=1S/C18H26ClNO4/c1-13(2)6-5-11-24-18(22)8-4-7-17(21)20-15-12-14(19)9-10-16(

InchiKey: HFYCAOMIOQGBEQ-UHFFFAOYSA-N

Formula: C18H26ClNO4

SMILES: COc1ccc(Cl)cc1NC(=O)CCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 355.86

Physical Properties

Property code	Value	Unit	Source
gf	-198.99	kJ/mol	Joback Method
hf	-658.41	kJ/mol	Joback Method
hfus	46.99	kJ/mol	Joback Method
hvap	88.01	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.437		Crippen Method
mcvol	277.820	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2969.00		NIST Webbook
rinpol	2969.00		NIST Webbook
tb	887.62	K	Joback Method
tc	1098.40	K	Joback Method
tf	555.98	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.32	J/mol×K	887.62	Joback Method
cpg	858.03	J/mol×K	922.75	Joback Method
cpg	870.57	J/mol×K	957.88	Joback Method
cpg	881.96	J/mol×K	993.01	Joback Method
cpg	892.23	J/mol×K	1028.14	Joback Method
cpg	901.39	J/mol×K	1063.27	Joback Method
cpg	909.46	J/mol×K	1098.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360756&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