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

Inchi: InChI=1S/C16H22ClNO4/c1-11(2)10-22-16(20)6-4-5-15(19)18-13-9-12(17)7-8-14(13)21-

InchiKey: QSMDKKFRZWCCTO-UHFFFAOYSA-N

Formula: C16H22ClNO4

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

Mol. weight [g/mol]: 327.80

Physical Properties

Property code	Value	Unit	Source
gf	-215.83	kJ/mol	Joback Method
hf	-617.13	kJ/mol	Joback Method
hfus	41.81	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.657		Crippen Method
mcvol	249.640	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	2742.00		NIST Webbook
tb	841.86	K	Joback Method
tc	1052.83	K	Joback Method
tf	533.44	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.47	J/mol×K	841.86	Joback Method
cpg	742.77	J/mol×K	877.02	Joback Method
cpg	755.00	J/mol×K	912.18	Joback Method
cpg	766.16	J/mol×K	947.34	Joback Method
cpg	776.27	J/mol×K	982.50	Joback Method
cpg	785.34	J/mol×K	1017.67	Joback Method
cpg	793.39	J/mol×K	1052.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360753&Units=SI

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