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

Inchi: InChI=1S/C16H22ClNO4/c1-3-4-10-22-16(20)7-5-6-15(19)18-13-11-12(17)8-9-14(13)21-

InchiKey: KDYIMGJCFBCQHH-UHFFFAOYSA-N

Formula: C16H22ClNO4

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

Mol. weight [g/mol]: 327.80

Physical Properties

Property code	Value	Unit	Source
gf	-213.39	kJ/mol	Joback Method
hf	-611.85	kJ/mol	Joback Method
hfus	45.33	kJ/mol	Joback Method
hvap	83.94	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.801		Crippen Method
mcvol	249.640	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2791.00		NIST Webbook
tb	842.30	K	Joback Method
tc	1050.93	K	Joback Method
tf	548.44	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.91	J/mol×K	842.30	Joback Method
cpg	742.08	J/mol×K	877.07	Joback Method
cpg	754.21	J/mol×K	911.84	Joback Method
cpg	765.31	J/mol×K	946.62	Joback Method
cpg	775.39	J/mol×K	981.39	Joback Method
cpg	784.47	J/mol×K	1016.16	Joback Method
cpg	792.56	J/mol×K	1050.93	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=U360754&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