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

Inchi: InChI=1S/C19H28ClNO4/c1-3-4-5-6-7-13-25-19(23)10-8-9-18(22)21-16-14-15(20)11-12-

InchiKey: HTPHMGFUMIZDJM-UHFFFAOYSA-N

Formula: C19H28ClNO4

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

Mol. weight [g/mol]: 369.88

Physical Properties

Property code	Value	Unit	Source
gf	-188.13	kJ/mol	Joback Method
hf	-673.77	kJ/mol	Joback Method
hfus	53.10	kJ/mol	Joback Method
hvap	90.62	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.971		Crippen Method
mcvol	291.910	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
rinpol	3108.00		NIST Webbook
tb	910.94	K	Joback Method
tc	1121.43	K	Joback Method
tf	582.25	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.36	J/mol×K	910.94	Joback Method
cpg	916.18	J/mol×K	946.02	Joback Method
cpg	928.82	J/mol×K	981.10	Joback Method
cpg	940.30	J/mol×K	1016.18	Joback Method
cpg	950.63	J/mol×K	1051.27	Joback Method
cpg	959.83	J/mol×K	1086.35	Joback Method
cpg	967.93	J/mol×K	1121.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360758&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