Glutaric acid, monoamide, N-(2-methoxybenzyl)-, ethyl ester

Inchi: InChI=1S/C15H21NO4/c1-3-20-15(18)10-6-9-14(17)16-11-12-7-4-5-8-13(12)19-2/h4-5,7-

InchiKey: YZDWVEKAOSYWDU-UHFFFAOYSA-N

Formula: C15H21NO4

SMILES: CCOC(=O)CCCC(=O)NCc1ccccc1OC

Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-200.25	kJ/mol	Joback Method
hf	-564.00	kJ/mol	Joback Method
hfus	38.93	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.045		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2336.00		NIST Webbook
tb	777.01	K	Joback Method
tc	981.78	K	Joback Method
tf	494.73	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.74	J/mol×K	777.01	Joback Method
cpg	662.86	J/mol×K	811.14	Joback Method
cpg	676.00	J/mol×K	845.27	Joback Method
cpg	688.16	J/mol×K	879.40	Joback Method
cpg	699.37	J/mol×K	913.52	Joback Method
cpg	709.63	J/mol×K	947.65	Joback Method
cpg	718.96	J/mol×K	981.78	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=U360023&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