Glutaric acid, monoamide, N-(4-methoxybenzyl)-, butyl ester

Inchi: InChI=1S/C17H25NO4/c1-3-4-12-22-17(20)7-5-6-16(19)18-13-14-8-10-15(21-2)11-9-14/h
InchiKey: PTJUDMWOXNBCBE-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: CCCCOC(=O)CCCC(=O)NCc1ccc(OC)cc1
Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
gf	-183.41	kJ/mol	Joback Method
hf	-605.28	kJ/mol	Joback Method
hfus	44.11	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.825		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2606.00		NIST Webbook
tb	822.77	K	Joback Method
tc	1025.84	K	Joback Method
tf	517.27	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.56	J/mol×K	822.77	Joback Method
cpg	776.21	J/mol×K	856.62	Joback Method
cpg	789.80	J/mol×K	890.46	Joback Method
cpg	802.35	J/mol×K	924.31	Joback Method
cpg	813.88	J/mol×K	958.15	Joback Method
cpg	824.40	J/mol×K	992.00	Joback Method
cpg	833.92	J/mol×K	1025.84	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=U360190&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