Glutaric acid, monoamide, N-butyl-N-phenyl-, ethyl ester

Inchi: InChI=1S/C17H25NO3/c1-3-5-14-18(15-10-7-6-8-11-15)16(19)12-9-13-17(20)21-4-2/h6-8

InchiKey: WLMLYKXEKLHMRA-UHFFFAOYSA-N

Formula: C17H25NO3

SMILES: CCCCN(C(=O)CCCC(=O)OCC)c1ccccc1

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-47.39	kJ/mol	Joback Method
hf	-447.53	kJ/mol	Joback Method
hfus	41.23	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.553		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook
tb	757.64	K	Joback Method
tc	956.43	K	Joback Method
tf	462.33	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.56	J/mol×K	757.64	Joback Method
cpg	733.54	J/mol×K	790.77	Joback Method
cpg	748.50	J/mol×K	823.90	Joback Method
cpg	762.47	J/mol×K	857.03	Joback Method
cpg	775.49	J/mol×K	890.16	Joback Method
cpg	787.61	J/mol×K	923.30	Joback Method
cpg	798.87	J/mol×K	956.43	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=U360169&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