Glutaric acid, monoamide, N-(2-phenylpropyl)-, butyl ester

Inchi: InChI=1S/C18H27NO3/c1-3-4-13-22-18(21)12-8-11-17(20)19-14-15(2)16-9-6-5-7-10-16/h
InchiKey: YWZNYQMTRPMFKV-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CCCCOC(=O)CCCC(=O)NCC(C)c1ccccc1
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-62.80	kJ/mol	Joback Method
hf	-487.51	kJ/mol	Joback Method
hfus	42.38	kJ/mol	Joback Method
hvap	79.89	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.420		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	2432.00		NIST Webbook
tb	817.81	K	Joback Method
tc	1021.72	K	Joback Method
tf	478.79	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.02	J/mol×K	817.81	Joback Method
cpg	807.59	J/mol×K	851.80	Joback Method
cpg	822.09	J/mol×K	885.78	Joback Method
cpg	835.54	J/mol×K	919.77	Joback Method
cpg	848.00	J/mol×K	953.75	Joback Method
cpg	859.49	J/mol×K	987.74	Joback Method
cpg	870.06	J/mol×K	1021.72	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=U360821&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