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

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

Physical Properties

Property code	Value	Unit	Source
gf	-38.97	kJ/mol	Joback Method
hf	-468.17	kJ/mol	Joback Method
hfus	43.82	kJ/mol	Joback Method
hvap	75.88	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.943		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	780.52	K	Joback Method
tc	978.42	K	Joback Method
tf	473.60	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.46	J/mol×K	780.52	Joback Method
cpg	790.69	J/mol×K	813.50	Joback Method
cpg	805.87	J/mol×K	846.49	Joback Method
cpg	820.05	J/mol×K	879.47	Joback Method
cpg	833.27	J/mol×K	912.45	Joback Method
cpg	845.57	J/mol×K	945.44	Joback Method
cpg	856.99	J/mol×K	978.42	Joback Method

Sources

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=U360170&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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