

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

Inchi:	InChI=1S/C19H29NO3/c1-3-5-15-20(17-11-8-7-9-12-17)18(21)13-10-14-19(22)23-16-6-4
InchiKey:	OQNSLRCDVTTZMA-UHFFFAOYSA-N
Formula:	C19H29NO3
SMILES:	CCCCOC(=O)CCCC(=O)N(CCCC)c1ccccc1
Mol. weight [g/mol]:	319.44

Physical Properties

Property code	Value	Unit	Source
gf	-30.55	kJ/mol	Joback Method
hf	-488.81	kJ/mol	Joback Method
hfus	46.41	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.333		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2343.00		NIST Webbook
rinpol	2343.00		NIST Webbook
tb	803.40	K	Joback Method
tc	1001.00	K	Joback Method
tf	484.87	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.30	J/mol×K	803.40	Joback Method
cpg	848.76	J/mol×K	836.33	Joback Method
cpg	864.15	J/mol×K	869.27	Joback Method
cpg	878.52	J/mol×K	902.20	Joback Method
cpg	891.91	J/mol×K	935.13	Joback Method
cpg	904.37	J/mol×K	968.07	Joback Method
cpg	915.94	J/mol×K	1001.00	Joback Method

Sources

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=U360172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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