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

Inchi: InChI=1S/C19H29NO3/c1-4-5-14-20(17-10-7-6-8-11-17)18(21)12-9-13-19(22)23-15-16(2

InchiKey: WLTQGFFRFDJYJJ-UHFFFAOYSA-N

Formula: C19H29NO3

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

Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	-32.99	kJ/mol	Joback Method
hf	-494.09	kJ/mol	Joback Method
hfus	42.89	kJ/mol	Joback Method
hvap	77.72	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.189		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
tb	802.96	K	Joback Method
tc	1002.69	K	Joback Method
tf	469.87	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.83	J/mol×K	802.96	Joback Method
cpg	849.46	J/mol×K	836.25	Joback Method
cpg	864.99	J/mol×K	869.54	Joback Method
cpg	879.47	J/mol×K	902.83	Joback Method
cpg	892.94	J/mol×K	936.11	Joback Method
cpg	905.45	J/mol×K	969.40	Joback Method
cpg	917.04	J/mol×K	1002.69	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=U360171&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/59-017-8/Glutaric-acid-monoamide-N-butyl-N-phenyl-isobutyl-ester.pdf
Generated by Cheméo on 2024-10-12 08:03:40.42578648 +0000 UTC m=+3301083.062755729.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.