

Glutaranilic acid, 3-[(phenylcarbamoyl)methyl]-

Inchi:	InChI=1S/C19H20N2O4/c22-17(20-15-7-3-1-4-8-15)11-14(13-19(24)25)12-18(23)21-16-9
InchiKey:	UMSKQABXUWPEIV-UHFFFAOYSA-N
Formula:	C19H20N2O4
SMILES:	O=C(O)CC(CC(=O)Nc1ccccc1)CC(=O)Nc1ccccc1
Mol. weight [g/mol]:	340.37

Physical Properties

Property code	Value	Unit	Source
gf	-13.32	kJ/mol	Joback Method
hf	-350.74	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	111.84	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.135		Crippen Method
mcvol	261.590	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
tb	1041.17	K	Joback Method
tc	1278.87	K	Joback Method
tf	657.66	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.22	J/molxK	1041.17	Joback Method
cpg	842.51	J/molxK	1080.79	Joback Method
cpg	850.94	J/molxK	1120.40	Joback Method
cpg	858.60	J/molxK	1160.02	Joback Method
cpg	865.61	J/molxK	1199.64	Joback Method
cpg	872.05	J/molxK	1239.25	Joback Method
cpg	878.03	J/molxK	1278.87	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=B6008227&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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