

Glutaric acid, monoamide, N-(1-phenylethyl)-, hexyl ester

Inchi:	InChI=1S/C19H29NO3/c1-3-4-5-9-15-23-19(22)14-10-13-18(21)20-16(2)17-11-7-6-8-12-
InchiKey:	YOJOWOXTYXLILF-UHFFFAOYSA-N
Formula:	C19H29NO3
SMILES:	CCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1
Mol. weight [g/mol]:	319.44

Physical Properties

Property code	Value	Unit	Source
gf	-54.38	kJ/mol	Joback Method
hf	-508.15	kJ/mol	Joback Method
hfus	44.97	kJ/mol	Joback Method
hvap	82.11	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.158		Crippen Method
mvol	273.800	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook
tb	840.69	K	Joback Method
tc	1044.46	K	Joback Method
tf	490.06	K	Joback Method
vc	1.050	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.20	J/mol×K	840.69	Joback Method
cpg	865.99	J/mol×K	874.65	Joback Method
cpg	880.66	J/mol×K	908.61	Joback Method
cpg	894.28	J/mol×K	942.58	Joback Method
cpg	906.87	J/mol×K	976.54	Joback Method
cpg	918.49	J/mol×K	1010.50	Joback Method
cpg	929.16	J/mol×K	1044.46	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=U360156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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