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

Inchi: InChI=1S/C15H21NO3/c1-3-19-15(18)11-7-10-14(17)16-12(2)13-8-5-4-6-9-13/h4-6,8-9,1

InchiKey: SKSMFOAJXXILTL-UHFFFAOYSA-N

Formula: C15H21NO3

SMILES: CCOC(=O)CCCC(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 263.33

Physical Properties

Property code	Value	Unit	Source
gf	-88.06	kJ/mol	Joback Method
hf	-425.59	kJ/mol	Joback Method
hfus	34.61	kJ/mol	Joback Method
hvap	73.21	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.597		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	2125.00		NIST Webbook
tb	749.17	K	Joback Method
tc	957.17	K	Joback Method
tf	444.98	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.92	J/mol×K	749.17	Joback Method
cpg	637.75	J/mol×K	783.84	Joback Method
cpg	651.56	J/mol×K	818.50	Joback Method
cpg	664.40	J/mol×K	853.17	Joback Method
cpg	676.28	J/mol×K	887.84	Joback Method
cpg	687.25	J/mol×K	922.50	Joback Method
cpg	697.34	J/mol×K	957.17	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=U360150&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

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