Glutaric acid, monoamide, N-(2-phenylpropyl)-, ethyl ester

Inchi: InChI=1S/C16H23NO3/c1-3-20-16(19)11-7-10-15(18)17-12-13(2)14-8-5-4-6-9-14/h4-6,8-

InchiKey: PLHFKBMYUJNBNO-UHFFFAOYSA-N

Formula: C16H23NO3

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

Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-79.64	kJ/mol	Joback Method
hf	-446.23	kJ/mol	Joback Method
hfus	37.20	kJ/mol	Joback Method
hvap	75.44	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.640		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	2234.00		NIST Webbook
tb	772.05	K	Joback Method
tc	978.12	K	Joback Method
tf	456.25	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.31	J/mol×K	772.05	Joback Method
cpg	693.41	J/mol×K	806.40	Joback Method
cpg	707.49	J/mol×K	840.74	Joback Method
cpg	720.56	J/mol×K	875.09	Joback Method
cpg	732.67	J/mol×K	909.43	Joback Method
cpg	743.85	J/mol×K	943.78	Joback Method
cpg	754.13	J/mol×K	978.12	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=U360818&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