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

Inchi: InChI=1S/C17H25NO3/c1-3-12-21-17(20)11-7-10-16(19)18-13-14(2)15-8-5-4-6-9-15/h4-

InchiKey: ACHOOMBRYHOMCZ-UHFFFAOYSA-N

Formula: C17H25NO3

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

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-71.22	kJ/mol	Joback Method
hf	-466.87	kJ/mol	Joback Method
hfus	39.79	kJ/mol	Joback Method
hvap	77.66	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.030		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	794.93	K	Joback Method
tc	999.63	K	Joback Method
tf	467.52	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.70	J/mol×K	794.93	Joback Method
cpg	750.05	J/mol×K	829.05	Joback Method
cpg	764.34	J/mol×K	863.16	Joback Method
cpg	777.62	J/mol×K	897.28	Joback Method
cpg	789.92	J/mol×K	931.39	Joback Method
cpg	801.27	J/mol×K	965.51	Joback Method
cpg	811.71	J/mol×K	999.63	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U360819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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