Glutaric acid, monoamide, N-(3-methylphenyl)-, propyl ester

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

InchiKey: XADFDUJIFAWKNQ-UHFFFAOYSA-N

Formula: C15H21NO3

SMILES: CCCOC(=O)CCCC(=O)Nc1cccc(C)c1

Mol. weight [g/mol]: 263.33

Physical Properties

Property code	Value	Unit	Source
gf	-95.25	kJ/mol	Joback Method
hf	-431.78	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	74.26	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.057		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	754.59	K	Joback Method
tc	960.29	K	Joback Method
tf	472.50	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.45	J/mol×K	754.59	Joback Method
cpg	635.94	J/mol×K	788.87	Joback Method
cpg	649.47	J/mol×K	823.16	Joback Method
cpg	662.07	J/mol×K	857.44	Joback Method
cpg	673.77	J/mol×K	891.72	Joback Method
cpg	684.59	J/mol×K	926.01	Joback Method
cpg	694.55	J/mol×K	960.29	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=U360913&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