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

Inchi: InChI=1S/C16H23NO3/c1-12(2)11-20-16(19)9-5-8-15(18)17-14-7-4-6-13(3)10-14/h4,6-7,
InchiKey: UWZLOTJUWFGONI-UHFFFAOYSA-N
Formula: C16H23NO3
SMILES: Cc1cccc(NC(=O)CCCC(=O)OCC(C)C)c1
Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-89.27	kJ/mol	Joback Method
hf	-457.70	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.303		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	2540.00		NIST Webbook
tb	777.03	K	Joback Method
tc	983.90	K	Joback Method
tf	468.77	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.44	J/mol×K	777.03	Joback Method
cpg	692.45	J/mol×K	811.51	Joback Method
cpg	706.43	J/mol×K	845.99	Joback Method
cpg	719.42	J/mol×K	880.46	Joback Method
cpg	731.45	J/mol×K	914.94	Joback Method
cpg	742.54	J/mol×K	949.42	Joback Method
cpg	752.73	J/mol×K	983.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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