Glutaric acid, monoamide, N-(4-methylbenzyl)-, butyl ester

Inchi: InChI=1S/C17H25NO3/c1-3-4-12-21-17(20)7-5-6-16(19)18-13-15-10-8-14(2)9-11-15/h8-1

InchiKey: WOLXXBVCNZGIRP-UHFFFAOYSA-N

Formula: C17H25NO3

SMILES: CCCCOC(=O)CCCC(=O)NCc1ccc(C)cc1

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-78.41	kJ/mol	Joback Method
hf	-473.06	kJ/mol	Joback Method
hfus	42.92	kJ/mol	Joback Method
hvap	78.71	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.125		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2447.00		NIST Webbook
tb	800.35	K	Joback Method
tc	1003.35	K	Joback Method
tf	495.04	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.33	J/mol×K	800.35	Joback Method
cpg	748.41	J/mol×K	834.18	Joback Method
cpg	762.47	J/mol×K	868.02	Joback Method
cpg	775.56	J/mol×K	901.85	Joback Method
cpg	787.69	J/mol×K	935.68	Joback Method
cpg	798.90	J/mol×K	969.52	Joback Method
cpg	809.22	J/mol×K	1003.35	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=U360011&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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