

Glutaric acid, monoamide, N-(4-ethylphenyl)-, pentyl ester

Inchi: InChI=1S/C18H27NO3/c1-3-5-6-14-22-18(21)9-7-8-17(20)19-16-12-10-15(4-2)11-13-16/
InchiKey: FVRQYOZKFMAFFF-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CCCCCOC(=O)CCCC(=O)Nc1ccc(CC)cc1
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-69.99	kJ/mol	Joback Method
hf	-493.70	kJ/mol	Joback Method
hfus	45.51	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.091		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2819.00		NIST Webbook
rinpol	2819.00		NIST Webbook
tb	823.23	K	Joback Method
tc	1025.77	K	Joback Method
tf	506.31	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.71	J/mol×K	823.23	Joback Method
cpg	806.04	J/mol×K	856.99	Joback Method
cpg	820.33	J/mol×K	890.74	Joback Method
cpg	833.61	J/mol×K	924.50	Joback Method
cpg	845.91	J/mol×K	958.26	Joback Method
cpg	857.27	J/mol×K	992.01	Joback Method
cpg	867.73	J/mol×K	1025.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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