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

Inchi: InChI=1S/C21H33NO3/c1-3-4-5-6-7-8-16-25-21(24)11-9-10-20(23)22-17-19-14-12-18(2)
InchiKey: VXIKTHDSVZKHLX-UHFFFAOYSA-N
Formula: C21H33NO3
SMILES: CCCCCCCCOC(=O)CCCC(=O)NCc1ccc(C)cc1
Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
gf	-44.73	kJ/mol	Joback Method
hf	-555.62	kJ/mol	Joback Method
hfus	53.28	kJ/mol	Joback Method
hvap	87.62	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.685		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2838.00		NIST Webbook
rinpol	2838.00		NIST Webbook
tb	891.87	K	Joback Method
tc	1097.18	K	Joback Method
tf	540.12	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.75	J/mol×K	891.87	Joback Method
cpg	983.80	J/mol×K	926.09	Joback Method
cpg	998.70	J/mol×K	960.31	Joback Method
cpg	1012.49	J/mol×K	994.52	Joback Method
cpg	1025.22	J/mol×K	1028.74	Joback Method
cpg	1036.92	J/mol×K	1062.96	Joback Method
cpg	1047.64	J/mol×K	1097.18	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=U360015&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