Glutaric acid, monoamide, N-(2-(4-methoxyphenyl)ethyl)-, heptyl ester

Inchi: InChI=1S/C21H33NO4/c1-3-4-5-6-7-17-26-21(24)10-8-9-20(23)22-16-15-18-11-13-19(25

InchiKey: BAHKJHWIGAOCKP-UHFFFAOYSA-N

Formula: C21H33NO4

SMILES: CCCCCCCOC(=O)CCCC(=O)NCCc1ccc(OC)cc1

Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
gf	-149.73	kJ/mol	Joback Method
hf	-687.84	kJ/mol	Joback Method
hfus	54.47	kJ/mol	Joback Method
hvap	90.03	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.038		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	2996.00		NIST Webbook
tb	914.29	K	Joback Method
tc	1122.24	K	Joback Method
tf	562.35	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.02	J/mol×K	914.29	Joback Method
cpg	1012.54	J/mol×K	948.95	Joback Method
cpg	1026.79	J/mol×K	983.61	Joback Method
cpg	1039.81	J/mol×K	1018.27	Joback Method
cpg	1051.64	J/mol×K	1052.92	Joback Method
cpg	1062.30	J/mol×K	1087.58	Joback Method
cpg	1071.81	J/mol×K	1122.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360223&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume