Glutaric acid, monoamide, N-(4-methoxybenzyl)-, hexyl ester

Inchi: InChI=1S/C19H29NO4/c1-3-4-5-6-14-24-19(22)9-7-8-18(21)20-15-16-10-12-17(23-2)13-

InchiKey: DMRNJYSUXBYEFU-UHFFFAOYSA-N

Formula: C19H29NO4

SMILES: CCCCCCOC(=O)CCCC(=O)NCc1ccc(OC)cc1

Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
gf	-166.57	kJ/mol	Joback Method
hf	-646.56	kJ/mol	Joback Method
hfus	49.29	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.605		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2795.00		NIST Webbook
rinpol	2795.00		NIST Webbook
tb	868.53	K	Joback Method
tc	1072.52	K	Joback Method
tf	539.81	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.84	J/mol×K	868.53	Joback Method
cpg	892.93	J/mol×K	902.53	Joback Method
cpg	906.88	J/mol×K	936.53	Joback Method
cpg	919.70	J/mol×K	970.53	Joback Method
cpg	931.42	J/mol×K	1004.53	Joback Method
cpg	942.05	J/mol×K	1038.52	Joback Method
cpg	951.64	J/mol×K	1072.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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