Glutaric acid, monoamide, N-(2-methoxybenzyl)-, heptyl ester

Inchi: InChI=1S/C20H31NO4/c1-3-4-5-6-9-15-25-20(23)14-10-13-19(22)21-16-17-11-7-8-12-18

InchiKey: VKKDQISNUJGZOH-UHFFFAOYSA-N

Formula: C20H31NO4

SMILES: CCCCCCCOC(=O)CCCC(=O)NCc1ccccc1OC

Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
gf	-158.15	kJ/mol	Joback Method
hf	-667.20	kJ/mol	Joback Method
hfus	51.88	kJ/mol	Joback Method
hvap	87.80	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.995		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2817.00		NIST Webbook
tb	891.41	K	Joback Method
tc	1096.98	K	Joback Method
tf	551.08	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.10	J/mol×K	891.41	Joback Method
cpg	952.40	J/mol×K	925.67	Joback Method
cpg	966.51	J/mol×K	959.93	Joback Method
cpg	979.43	J/mol×K	994.19	Joback Method
cpg	991.21	J/mol×K	1028.45	Joback Method
cpg	1001.87	J/mol×K	1062.71	Joback Method
cpg	1011.44	J/mol×K	1096.98	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=U360030&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

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