Glutaric acid, monoamide, N-dodecyl-, isobutyl ester

Inchi: InChI=1S/C21H41NO3/c1-4-5-6-7-8-9-10-11-12-13-17-22-20(23)15-14-16-21(24)25-18-1

InchiKey: ZVRLDWZTBXPKEI-UHFFFAOYSA-N

Formula: C21H41NO3

SMILES: CCCCCCCCCCCCNC(=O)CCCC(=O)OCC(C)C

Mol. weight [g/mol]: 355.56

Physical Properties

Property code	Value	Unit	Source
gf	-149.95	kJ/mol	Joback Method
hf	-785.96	kJ/mol	Joback Method
hfus	56.11	kJ/mol	Joback Method
hvap	84.29	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.393		Crippen Method
mcvol	325.740	ml/mol	McGowan Method
pc	1037.90	kPa	Joback Method
rinpol	3074.00		NIST Webbook
tb	859.77	K	Joback Method
tc	1053.02	K	Joback Method
tf	486.18	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.06	J/mol×K	859.77	Joback Method
cpg	1082.62	J/mol×K	891.98	Joback Method
cpg	1100.03	J/mol×K	924.19	Joback Method
cpg	1116.34	J/mol×K	956.39	Joback Method
cpg	1131.57	J/mol×K	988.60	Joback Method
cpg	1145.76	J/mol×K	1020.81	Joback Method
cpg	1158.95	J/mol×K	1053.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360867&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