Glutaric acid, monoamide, N-(2-octyl)-, isobutyl ester

Inchi: InChI=1S/C17H33NO3/c1-5-6-7-8-10-15(4)18-16(19)11-9-12-17(20)21-13-14(2)3/h14-15

InchiKey: RCRKWAGXUSJUTA-UHFFFAOYSA-N

Formula: C17H33NO3

SMILES: CCCCCCC(C)NC(=O)CCCC(=O)OCC(C)C

Mol. weight [g/mol]: 299.45

Physical Properties

Property code	Value	Unit	Source
gf	-186.07	kJ/mol	Joback Method
hf	-708.68	kJ/mol	Joback Method
hfus	42.22	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.831		Crippen Method
mcvol	269.380	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2502.00		NIST Webbook
tb	767.81	K	Joback Method
tc	951.88	K	Joback Method
tf	426.10	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.82	J/mol×K	767.81	Joback Method
cpg	840.93	J/mol×K	798.49	Joback Method
cpg	857.10	J/mol×K	829.17	Joback Method
cpg	872.35	J/mol×K	859.84	Joback Method
cpg	886.69	J/mol×K	890.52	Joback Method
cpg	900.16	J/mol×K	921.20	Joback Method
cpg	912.77	J/mol×K	951.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360852&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