Glutaric acid, monoamide, N-(3-pentyl)-, isohexyl ester

Inchi: InChI=1S/C16H31NO3/c1-5-14(6-2)17-15(18)10-7-11-16(19)20-12-8-9-13(3)4/h13-14H,5

InchiKey: KFOMTYCXPIAJFQ-UHFFFAOYSA-N

Formula: C16H31NO3

SMILES: CCC(CC)NC(=O)CCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 285.42

Physical Properties

Property code	Value	Unit	Source
gf	-194.49	kJ/mol	Joback Method
hf	-688.04	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	72.77	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.441		Crippen Method
mcvol	255.290	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	2071.00		NIST Webbook
tb	744.93	K	Joback Method
tc	928.31	K	Joback Method
tf	414.83	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.84	J/mol×K	744.93	Joback Method
cpg	782.60	J/mol×K	775.49	Joback Method
cpg	798.46	J/mol×K	806.06	Joback Method
cpg	813.43	J/mol×K	836.62	Joback Method
cpg	827.53	J/mol×K	867.19	Joback Method
cpg	840.80	J/mol×K	897.75	Joback Method
cpg	853.24	J/mol×K	928.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360810&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

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