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

Inchi: InChI=1S/C17H33NO3/c1-4-7-8-9-10-14-21-17(20)13-11-12-16(19)18-15(5-2)6-3/h15H,4
InchiKey: FXXNFCCKCPDHHR-UHFFFAOYSA-N
Formula: C17H33NO3
SMILES: CCCCCCCOC(=O)CCCC(=O)NC(CC)CC
Mol. weight [g/mol]: 299.45

Physical Properties

Property code	Value	Unit	Source
gf	-183.63	kJ/mol	Joback Method
hf	-703.40	kJ/mol	Joback Method
hfus	45.75	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.975		Crippen Method
mcvol	269.380	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2208.00		NIST Webbook
tb	768.25	K	Joback Method
tc	950.75	K	Joback Method
tf	441.10	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.32	J/mol×K	768.25	Joback Method
cpg	840.28	J/mol×K	798.67	Joback Method
cpg	856.32	J/mol×K	829.08	Joback Method
cpg	871.45	J/mol×K	859.50	Joback Method
cpg	885.72	J/mol×K	889.92	Joback Method
cpg	899.12	J/mol×K	920.33	Joback Method
cpg	911.70	J/mol×K	950.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360812&Units=SI

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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