5-Cyano-2,3,3-pentanetricarboxylic acid, triethyl ester

Inchi: InChI=1S/C15H23NO6/c1-5-20-12(17)11(4)15(9-8-10-16,13(18)21-6-2)14(19)22-7-3/h11

InchiKey: SIMLAXQBSRSEKJ-UHFFFAOYSA-N

Formula: C15H23NO6

SMILES: CCOC(=O)C(C)C(CCC#N)(C(=O)OCC)C(=O)OCC

Mol. weight [g/mol]: 313.35

CAS: 3228-31-7

Physical Properties

Property code	Value	Unit	Source
gf	-492.76	kJ/mol	Joback Method
hf	-936.48	kJ/mol	Joback Method
hfus	33.54	kJ/mol	Joback Method
hvap	85.25	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.602		Crippen Method
mcvol	245.910	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
tb	869.88	K	Joback Method
tc	1076.75	K	Joback Method
tf	527.70	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.40	J/mol×K	869.88	Joback Method
cpg	766.39	J/mol×K	904.36	Joback Method
cpg	777.33	J/mol×K	938.84	Joback Method
cpg	787.25	J/mol×K	973.31	Joback Method
cpg	796.16	J/mol×K	1007.79	Joback Method
cpg	804.06	J/mol×K	1042.27	Joback Method
cpg	810.96	J/mol×K	1076.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3228317&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume