Cyanoacetic acid, heptyl ester

Inchi: InChI=1S/C10H17NO2/c1-2-3-4-5-6-9-13-10(12)7-8-11/h2-7,9H2,1H3
InchiKey: SJDCJXRWNRXTNZ-UHFFFAOYSA-N
Formula: C10H17NO2
SMILES: CCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 183.25

Physical Properties

Property code	Value	Unit	Source
gf	-67.42	kJ/mol	Joback Method
hf	-329.65	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	57.49	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.414		Crippen Method
mcvol	160.580	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1448.00		NIST Webbook
tb	606.57	K	Joback Method
tc	794.85	K	Joback Method
tf	339.61	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.48	J/mol×K	606.57	Joback Method
cpg	415.84	J/mol×K	637.95	Joback Method
cpg	427.63	J/mol×K	669.33	Joback Method
cpg	438.86	J/mol×K	700.71	Joback Method
cpg	449.54	J/mol×K	732.09	Joback Method
cpg	459.68	J/mol×K	763.47	Joback Method
cpg	469.27	J/mol×K	794.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406224&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