Undec-10-ynoic acid, propyl ester

Inchi: InChI=1S/C14H24O2/c1-3-5-6-7-8-9-10-11-12-14(15)16-13-4-2/h1H,4-13H2,2H3
InchiKey: NTWOHKRWOQBBJB-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: C#CCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	56.15	kJ/mol	Joback Method
hf	-285.19	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	55.77	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.694		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	586.13	K	Joback Method
tc	762.74	K	Joback Method
tf	366.67	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.73	J/mol×K	586.13	Joback Method
cpg	540.68	J/mol×K	615.57	Joback Method
cpg	555.94	J/mol×K	645.00	Joback Method
cpg	570.52	J/mol×K	674.44	Joback Method
cpg	584.44	J/mol×K	703.87	Joback Method
cpg	597.71	J/mol×K	733.31	Joback Method
cpg	610.36	J/mol×K	762.74	Joback Method

Sources

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=U406155&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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