Undec-10-ynoic acid, tridec-2-yn-1-yl ester

Inchi: InChI=1S/C24H40O2/c1-3-5-7-9-11-13-14-15-17-19-21-23-26-24(25)22-20-18-16-12-10-
InchiKey: KNSRYXHYKIDPGF-UHFFFAOYSA-N
Formula: C24H40O2
SMILES: C#CCCCCCCCCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]: 360.57

Physical Properties

Property code	Value	Unit	Source
gf	343.15	kJ/mol	Joback Method
hf	-219.29	kJ/mol	Joback Method
hfus	66.80	kJ/mol	Joback Method
hvap	80.18	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	6.818		Crippen Method
mcvol	339.260	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	2637.00		NIST Webbook
rinpol	2637.00		NIST Webbook
tb	823.93	K	Joback Method
tc	1013.92	K	Joback Method
tf	585.47	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.54	J/mol×K	823.93	Joback Method
cpg	1070.03	J/mol×K	855.59	Joback Method
cpg	1088.47	J/mol×K	887.26	Joback Method
cpg	1105.91	J/mol×K	918.92	Joback Method
cpg	1122.37	J/mol×K	950.59	Joback Method
cpg	1137.91	J/mol×K	982.25	Joback Method
cpg	1152.56	J/mol×K	1013.92	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=U406969&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