Undec-10-ynoic acid, tetradecyl ester

Inchi: InChI=1S/C25H46O2/c1-3-5-7-9-11-13-14-15-16-18-20-22-24-27-25(26)23-21-19-17-12-
InchiKey: AGXFKXFGJDTHNJ-UHFFFAOYSA-N
Formula: C25H46O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 378.63

Physical Properties

Property code	Value	Unit	Source
gf	148.77	kJ/mol	Joback Method
hf	-512.23	kJ/mol	Joback Method
hfus	66.27	kJ/mol	Joback Method
hvap	80.26	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.985		Crippen Method
mcvol	361.950	ml/mol	McGowan Method
pc	852.97	kPa	Joback Method
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
tb	837.81	K	Joback Method
tc	1025.90	K	Joback Method
tf	490.64	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.34	J/mol×K	837.81	Joback Method
cpg	1183.27	J/mol×K	869.16	Joback Method
cpg	1203.07	J/mol×K	900.51	Joback Method
cpg	1221.78	J/mol×K	931.85	Joback Method
cpg	1239.46	J/mol×K	963.20	Joback Method
cpg	1256.14	J/mol×K	994.55	Joback Method
cpg	1271.87	J/mol×K	1025.90	Joback Method

Sources

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=U406167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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