Undec-10-ynoic acid, dodecyl ester

Inchi: InChI=1S/C23H42O2/c1-3-5-7-9-11-13-14-16-18-20-22-25-23(24)21-19-17-15-12-10-8-6
InchiKey: CPUMHCZZUYHHHY-UHFFFAOYSA-N
Formula: C23H42O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 350.58

Physical Properties

Property code	Value	Unit	Source
gf	131.93	kJ/mol	Joback Method
hf	-470.95	kJ/mol	Joback Method
hfus	61.09	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.205		Crippen Method
mcvol	333.770	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	2409.00		NIST Webbook
rinpol	2409.00		NIST Webbook
tb	792.05	K	Joback Method
tc	972.64	K	Joback Method
tf	468.10	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.43	J/mol×K	792.05	Joback Method
cpg	1057.38	J/mol×K	822.15	Joback Method
cpg	1076.31	J/mol×K	852.25	Joback Method
cpg	1094.27	J/mol×K	882.35	Joback Method
cpg	1111.28	J/mol×K	912.45	Joback Method
cpg	1127.39	J/mol×K	942.55	Joback Method
cpg	1142.63	J/mol×K	972.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406165&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume