3-Methyl-2-butenoic acid, undec-2-enyl ester

Inchi: InChI=1S/C16H28O2/c1-4-5-6-7-8-9-10-11-12-13-18-16(17)14-15(2)3/h11-12,14H,4-10,1
InchiKey: DWOVFZMUPZHBTN-VAWYXSNFSA-N
Formula: C16H28O2
SMILES: CCCCCCCCC=CCOC(=O)C=C(C)C
Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	1.81	kJ/mol	Joback Method
hf	-393.72	kJ/mol	Joback Method
hfus	39.08	kJ/mol	Joback Method
hvap	60.36	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.803		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	649.97	K	Joback Method
tc	830.08	K	Joback Method
tf	318.12	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.83	J/mol×K	649.97	Joback Method
cpg	651.07	J/mol×K	679.99	Joback Method
cpg	667.50	J/mol×K	710.01	Joback Method
cpg	683.13	J/mol×K	740.02	Joback Method
cpg	698.02	J/mol×K	770.04	Joback Method
cpg	712.19	J/mol×K	800.06	Joback Method
cpg	725.69	J/mol×K	830.08	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=U299316&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