

Butanoic acid, undec-2-enyl ester

Inchi:	InChI=1S/C15H28O2/c1-3-5-6-7-8-9-10-11-12-14-17-15(16)13-4-2/h11-12H,3-10,13-14H
InchiKey:	YKKKIRWPZWWRHL-VAWYXSNFSA-N
Formula:	C15H28O2
SMILES:	CCCCCCCCC=CCOC(=O)CCC
Mol. weight [g/mol]:	240.38

Physical Properties

Property code	Value	Unit	Source
gf	-78.28	kJ/mol	Joback Method
hf	-480.51	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	58.10	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.636		Crippen Method
mvol	225.350	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	1663.00		NIST Webbook
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tb	623.05	K	Joback Method
tc	796.03	K	Joback Method
tf	325.89	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.59	J/mol×K	623.05	Joback Method
cpg	617.60	J/mol×K	651.88	Joback Method
cpg	633.86	J/mol×K	680.71	Joback Method
cpg	649.40	J/mol×K	709.54	Joback Method
cpg	664.23	J/mol×K	738.37	Joback Method
cpg	678.37	J/mol×K	767.20	Joback Method
cpg	691.85	J/mol×K	796.03	Joback Method
dvisc	0.0024199	Paxs	325.89	Joback Method

dvisc	0.0010480	Paxs	375.42	Joback Method
dvisc	0.0005516	Paxs	424.94	Joback Method
dvisc	0.0003319	Paxs	474.47	Joback Method
dvisc	0.0002199	Paxs	524.00	Joback Method
dvisc	0.0001564	Paxs	573.52	Joback Method
dvisc	0.0001174	Paxs	623.05	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=U299125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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