

(E)-Dodec-2-enyl (E)-2-methylbut-2-enoate

Inchi:	InChI=1S/C17H30O2/c1-4-6-7-8-9-10-11-12-13-14-15-19-17(18)16(3)5-2/h5,13-14H,4,6-
InchiKey:	QAZZZLZNXNKS-NSIMVMACSA-N
Formula:	C17H30O2
SMILES:	CC=C(C)C(=O)OCC=CCCCCCCCC
Mol. weight [g/mol]:	266.42

Physical Properties

Property code	Value	Unit	Source
gf	10.23	kJ/mol	Joback Method
hf	-414.36	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.193		Crippen Method
mvol	249.230	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	1930.00		NIST Webbook
tb	672.85	K	Joback Method
tc	852.12	K	Joback Method
tf	329.39	K	Joback Method
vc	0.973	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.06	J/mol×K	672.85	Joback Method
cpg	706.70	J/mol×K	702.73	Joback Method
cpg	723.51	J/mol×K	732.61	Joback Method
cpg	739.52	J/mol×K	762.49	Joback Method
cpg	754.76	J/mol×K	792.37	Joback Method
cpg	769.27	J/mol×K	822.25	Joback Method
cpg	783.09	J/mol×K	852.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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