

(Z)-Dec-4-enyl (E)-2-methylbut-2-enoate

Inchi:	InChI=1S/C15H26O2/c1-4-6-7-8-9-10-11-12-13-17-15(16)14(3)5-2/h5,9-10H,4,6-8,11-13
InchiKey:	GNDJJJRLHIKVRW-DVBADTPPSA-N
Formula:	C15H26O2
SMILES:	CC=C(C)C(=O)OCCCC=CCCCC
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-6.61	kJ/mol	Joback Method
hf	-373.08	kJ/mol	Joback Method
hfus	36.49	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.412		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1703.00		NIST Webbook
tb	627.09	K	Joback Method
tc	808.40	K	Joback Method
tf	306.85	K	Joback Method
vc	0.861	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.91	J/mol×K	627.09	Joback Method
cpg	596.71	J/mol×K	657.31	Joback Method
cpg	612.71	J/mol×K	687.53	Joback Method
cpg	627.95	J/mol×K	717.74	Joback Method
cpg	642.45	J/mol×K	747.96	Joback Method
cpg	656.25	J/mol×K	778.18	Joback Method
cpg	669.38	J/mol×K	808.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373749&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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