

(S)-2-Methylbutyl (E)-7,9-decadienoate

Inchi:	InChI=1S/C15H26O2/c1-4-6-7-8-9-10-11-12-15(16)17-13-14(3)5-2/h4,6-7,14H,1,5,8-13H
InchiKey:	FPVAIPSGPXYQND-PSKZRQQASA-N
Formula:	C15H26O2
SMILES:	C=CC=CCCCCCC(=O)OCC(C)CC
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	7.12	kJ/mol	Joback Method
hf	-360.36	kJ/mol	Joback Method
hfus	32.79	kJ/mol	Joback Method
hvap	57.04	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.268		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	1676.00		NIST Webbook
tb	619.29	K	Joback Method
tc	797.56	K	Joback Method
tf	309.13	K	Joback Method
vc	0.855	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.91	J/molxK	619.29	Joback Method
cpg	655.44	J/molxK	767.84	Joback Method
cpg	641.60	J/molxK	738.13	Joback Method
cpg	627.06	J/molxK	708.42	Joback Method
cpg	611.78	J/molxK	678.71	Joback Method
cpg	595.74	J/molxK	649.00	Joback Method
cpg	668.59	J/molxK	797.56	Joback Method
dvisc	0.0001140	Paxs	619.29	Joback Method
dvisc	0.0001539	Paxs	567.60	Joback Method

dvisc	0.0002207	Paxs	515.90	Joback Method
dvisc	0.0003427	Paxs	464.21	Joback Method
dvisc	0.0005945	Paxs	412.52	Joback Method
dvisc	0.0012073	Paxs	360.82	Joback Method
dvisc	0.0031075	Paxs	309.13	Joback Method

Sources

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=R556628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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