

Allyl behenoate

Inchi:	InChI=1S/C25H48O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25(26
InchiKey:	VNVRAKHWAVVIGF-UHFFFAOYSA-N
Formula:	C25H48O2
SMILES:	C=CCOC(=O)CCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	380.65

Physical Properties

Property code	Value	Unit	Source
gf	13.54	kJ/mol	Joback Method
hf	-678.70	kJ/mol	Joback Method
hfus	62.01	kJ/mol	Joback Method
hvap	79.73	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	8.537		Crippen Method
mcvol	366.250	ml/mol	McGowan Method
pc	802.51	kPa	Joback Method
rinpol	2654.00		NIST Webbook
rinpol	2654.00		NIST Webbook
tb	844.37	K	Joback Method
tc	1033.82	K	Joback Method
tf	441.91	K	Joback Method
vc	1.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.62	J/molxK	844.37	Joback Method
cpg	1214.26	J/molxK	875.94	Joback Method
cpg	1234.69	J/molxK	907.52	Joback Method
cpg	1253.98	J/molxK	939.09	Joback Method
cpg	1272.17	J/molxK	970.67	Joback Method
cpg	1289.29	J/molxK	1002.24	Joback Method
cpg	1305.41	J/molxK	1033.82	Joback Method
dvisc	0.0009493	Paxs	441.91	Joback Method

dvisc	0.0003918	Paxs	508.99	Joback Method
dvisc	0.0001987	Paxs	576.06	Joback Method
dvisc	0.0001161	Paxs	643.14	Joback Method
dvisc	0.0000751	Paxs	710.22	Joback Method
dvisc	0.0000524	Paxs	777.29	Joback Method
dvisc	0.0000387	Paxs	844.37	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=R541116&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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