9,12,15-Octadecatrienoic acid, phenylmethyl ester, (z,z,z)-

Other names: Benzyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate
Linolenic acid, phenylmethyl ester
Benzyl linolenate

Inchi: InChI=1S/C25H36O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-25(26)27-23-24-20-17

InchiKey: XOMBABWFKFXLII-PDBXOOCHSA-N

Formula: C25H36O2

SMILES: CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)OCc1ccccc1

Mol. weight [g/mol]: 368.56

Physical Properties

Property code	Value	Unit	Source
hfus	57.94	kJ/mol	Joback Method
hvap	120.92	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.47		Cheméo Relay (1.0)
logp	7.319		Crippen Method
mcvol	333.890	ml/mol	McGowan Method
rinpol	2774.90		NIST Webbook
rinpol	2702.00		NIST Webbook
rinpol	2774.90		NIST Webbook
tb	642.35	K	Cheméo Relay (1.0)
tc	863.22	K	Cheméo Relay (1.0)
tf	257.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.54	J/mol×K	886.85	Joback Method
cpg	1146.73	J/mol×K	1092.88	Joback Method
cpg	1132.33	J/mol×K	1058.54	Joback Method
cpg	1117.33	J/mol×K	1024.21	Joback Method
cpg	1101.65	J/mol×K	989.87	Joback Method
cpg	1085.18	J/mol×K	955.53	Joback Method
cpg	1067.85	J/mol×K	921.19	Joback Method
dvisc	0.0000732	Pa×s	670.85	Joback Method

dvisc	0.0000247	Pa×s	886.85	Joback Method
dvisc	0.0000333	Pa×s	814.85	Joback Method
dvisc	0.0000475	Pa×s	742.85	Joback Method
dvisc	0.0006100	Pa×s	454.85	Joback Method
dvisc	0.0001252	Pa×s	598.85	Joback Method
dvisc	0.0002480	Pa×s	526.85	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77509025&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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