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: CCC=CCC=CCC=CCCCCCCCC(=O)OCc1ccccc1

Mol. weight [g/mol]: 368.55

CAS: 77509-02-5

Physical Properties

Property code	Value	Unit	Source
gf	278.77	kJ/mol	Joback Method
hf	-215.94	kJ/mol	Joback Method
hfus	57.94	kJ/mol	Joback Method
hvap	82.55	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.319		Crippen Method
mcvol	333.890	ml/mol	McGowan Method
pc	1050.73	kPa	Joback Method
rinpol	2774.90		NIST Webbook
rinpol	2702.00		NIST Webbook
tb	886.85	K	Joback Method
tc	1092.88	K	Joback Method
tf	454.85	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.54	J/mol×K	886.85	Joback Method
cpg	1067.85	J/mol×K	921.19	Joback Method
cpg	1085.18	J/mol×K	955.53	Joback Method
cpg	1101.65	J/mol×K	989.87	Joback Method

cpg	1117.33	J/mol×K	1024.21	Joback Method
cpg	1132.33	J/mol×K	1058.54	Joback Method
cpg	1146.73	J/mol×K	1092.88	Joback Method
dvisc	0.0006100	Pa×s	454.85	Joback Method
dvisc	0.0002480	Pa×s	526.85	Joback Method
dvisc	0.0001252	Pa×s	598.85	Joback Method
dvisc	0.0000732	Pa×s	670.85	Joback Method
dvisc	0.0000475	Pa×s	742.85	Joback Method
dvisc	0.0000333	Pa×s	814.85	Joback Method
dvisc	0.0000247	Pa×s	886.85	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=C77509025&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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