9,12-Octadecadienoic acid (Z,Z)-, phenylmethyl ester

Other names: Benzyl (9Z,12Z)-9,12-octadecadienoate
Linoleic acid, phenylmethyl ester
Benzyl linoleate
Dermol 618

Inchi: InChI=1S/C25H38O2/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: YDTIDQXHYVFIKB-HZJYTTRNSA-N

Formula: C25H38O2

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

Mol. weight [g/mol]: 370.57

CAS: 47557-83-5

Physical Properties

Property code	Value	Unit	Source
gf	198.55	kJ/mol	Joback Method
hf	-333.16	kJ/mol	Joback Method
hfus	57.74	kJ/mol	Joback Method
hvap	82.59	kJ/mol	Joback Method
log10ws	-8.46		Crippen Method
logp	7.543		Crippen Method
mcvol	338.190	ml/mol	McGowan Method
pc	1016.18	kPa	Joback Method
rinpol	2764.50		NIST Webbook
rinpol	2764.50		NIST Webbook
tb	882.69	K	Joback Method
tc	1085.61	K	Joback Method
tf	459.93	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.48	J/mol×K	882.69	Joback Method
cpg	1160.12	J/mol×K	1051.79	Joback Method
cpg	1145.19	J/mol×K	1017.97	Joback Method

cpg	1129.44	J/mol×K	984.15	Joback Method
cpg	1112.79	J/mol×K	950.33	Joback Method
cpg	1095.17	J/mol×K	916.51	Joback Method
cpg	1174.31	J/mol×K	1085.61	Joback Method
dvisc	0.0000282	Pa×s	882.69	Joback Method
dvisc	0.0000380	Pa×s	812.23	Joback Method
dvisc	0.0000541	Pa×s	741.77	Joback Method
dvisc	0.0000829	Pa×s	671.31	Joback Method
dvisc	0.0001404	Pa×s	600.85	Joback Method
dvisc	0.0002737	Pa×s	530.39	Joback Method
dvisc	0.0006544	Pa×s	459.93	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C47557835&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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