(9Z,12Z)-Phenethyl octadeca-9,12-dienoate

Inchi: InChI=1S/C26H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-26(27)28-24-23-25-20
InchiKey: QUEAXLYDBBSTME-HZJYTTRNSA-N
Formula: C26H40O2
SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	206.97	kJ/mol	Joback Method
hf	-353.80	kJ/mol	Joback Method
hfus	60.33	kJ/mol	Joback Method
hvap	84.82	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	7.586		Crippen Method
mcvol	352.280	ml/mol	McGowan Method
pc	956.73	kPa	Joback Method
rinpol	2864.40		NIST Webbook
rinpol	2864.40		NIST Webbook
tb	905.57	K	Joback Method
tc	1111.08	K	Joback Method
tf	471.20	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1138.59	J/mol×K	905.57	Joback Method
cpg	1223.87	J/mol×K	1076.83	Joback Method
cpg	1208.63	J/mol×K	1042.58	Joback Method
cpg	1192.56	J/mol×K	1008.33	Joback Method
cpg	1175.59	J/mol×K	974.07	Joback Method
cpg	1157.63	J/mol×K	939.82	Joback Method
cpg	1238.37	J/mol×K	1111.08	Joback Method
dvisc	0.0000244	Pa×s	905.57	Joback Method

dvisc	0.0000329	Pa×s	833.17	Joback Method
dvisc	0.0000470	Pa×s	760.78	Joback Method
dvisc	0.0000723	Pa×s	688.38	Joback Method
dvisc	0.0001230	Pa×s	615.99	Joback Method
dvisc	0.0002411	Pa×s	543.60	Joback Method
dvisc	0.0005810	Pa×s	471.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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