2-Phenoxyethyl pentadecanoate

Inchi: InChI=1S/C23H38O3/c1-2-3-4-5-6-7-8-9-10-11-12-16-19-23(24)26-21-20-25-22-17-14-13
InchiKey: JBDLVZUAMGDPCD-UHFFFAOYSA-N
Formula: C23H38O3
SMILES: CCCCCCCCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 362.55

Physical Properties

Property code	Value	Unit	Source
gf	-83.73	kJ/mol	Joback Method
hf	-658.54	kJ/mol	Joback Method
hfus	53.34	kJ/mol	Joback Method
hvap	80.63	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.700		Crippen Method
mcvol	324.480	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	2650.00		NIST Webbook
tb	851.03	K	Joback Method
tc	1046.21	K	Joback Method
tf	469.78	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.81	J/mol×K	851.03	Joback Method
cpg	1056.42	J/mol×K	883.56	Joback Method
cpg	1073.83	J/mol×K	916.09	Joback Method
cpg	1090.07	J/mol×K	948.62	Joback Method
cpg	1105.17	J/mol×K	981.15	Joback Method
cpg	1119.17	J/mol×K	1013.68	Joback Method
cpg	1132.11	J/mol×K	1046.21	Joback Method
dvisc	0.0006445	Pa×s	469.78	Joback Method
dvisc	0.0003012	Pa×s	533.32	Joback Method

dvisc	0.0001655	Pa×s	596.86	Joback Method
dvisc	0.0001020	Pa×s	660.40	Joback Method
dvisc	0.0000685	Pa×s	723.95	Joback Method
dvisc	0.0000490	Pa×s	787.49	Joback Method
dvisc	0.0000369	Pa×s	851.03	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=R540866&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