

2-Phenoxyethyl palmitate

Inchi:	InChI=1S/C24H40O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-24(25)27-22-21-26-23-18-15
InchiKey:	APJHZEOSLFDNDBG-UHFFFAOYSA-N
Formula:	C24H40O3
SMILES:	CCCCCCCCCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	376.57

Physical Properties

Property code	Value	Unit	Source
gf	-75.31	kJ/mol	Joback Method
hf	-679.18	kJ/mol	Joback Method
hfus	55.93	kJ/mol	Joback Method
hvap	82.86	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.090		Crippen Method
mcvol	338.570	ml/mol	McGowan Method
pc	1000.18	kPa	Joback Method
rinsol	2744.00		NIST Webbook
tb	873.91	K	Joback Method
tc	1071.92	K	Joback Method
tf	481.05	K	Joback Method
vc	1.313	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.54	J/molxK	873.91	Joback Method
cpg	1118.42	J/molxK	906.91	Joback Method
cpg	1136.04	J/molxK	939.91	Joback Method
cpg	1152.43	J/molxK	972.91	Joback Method
cpg	1167.65	J/molxK	1005.91	Joback Method
cpg	1181.72	J/molxK	1038.92	Joback Method
cpg	1194.68	J/molxK	1071.92	Joback Method
dvisc	0.0005745	Paxs	481.05	Joback Method
dvisc	0.0002659	Paxs	546.53	Joback Method

dvisc	0.0001451	Paxs	612.00	Joback Method
dvisc	0.0000890	Paxs	677.48	Joback Method
dvisc	0.0000595	Paxs	742.96	Joback Method
dvisc	0.0000425	Paxs	808.43	Joback Method
dvisc	0.0000319	Paxs	873.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540851&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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