

2-Phenoxyethyl heptanoate

Inchi:	InChI=1S/C15H22O3/c1-2-3-4-8-11-15(16)18-13-12-17-14-9-6-5-7-10-14/h5-7,9-10H,2-4
InchiKey:	SYCCMBAXMWVEES-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	CCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	250.33

Physical Properties

Property code	Value	Unit	Source
gf	-151.09	kJ/mol	Joback Method
hf	-493.42	kJ/mol	Joback Method
hfus	32.62	kJ/mol	Joback Method
hvap	62.83	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.579		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinsol	1816.00		NIST Webbook
tb	667.99	K	Joback Method
tc	864.11	K	Joback Method
tf	379.62	K	Joback Method
vc	0.809	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.40	J/molxK	667.99	Joback Method
cpg	647.51	J/molxK	831.42	Joback Method
cpg	634.65	J/molxK	798.73	Joback Method
cpg	620.93	J/molxK	766.05	Joback Method
cpg	606.32	J/molxK	733.36	Joback Method
cpg	590.82	J/molxK	700.68	Joback Method
cpg	659.52	J/molxK	864.11	Joback Method
dvisc	0.0001064	Paxs	667.99	Joback Method
dvisc	0.0001381	Paxs	619.93	Joback Method

dvisc	0.0001873	Paxs	571.87	Joback Method
dvisc	0.0002686	Paxs	523.81	Joback Method
dvisc	0.0004143	Paxs	475.74	Joback Method
dvisc	0.0007044	Paxs	427.68	Joback Method
dvisc	0.0013698	Paxs	379.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540826&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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