

2-Phenoxyethyl tridecanoate

Inchi:	InChI=1S/C21H34O3/c1-2-3-4-5-6-7-8-9-10-14-17-21(22)24-19-18-23-20-15-12-11-13-16
InchiKey:	YMEKRLRLRCVBNJW-UHFFFAOYSA-N
Formula:	C21H34O3
SMILES:	CCCCCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	334.49

Physical Properties

Property code	Value	Unit	Source
gf	-100.57	kJ/mol	Joback Method
hf	-617.26	kJ/mol	Joback Method
hfus	48.16	kJ/mol	Joback Method
hvap	76.18	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.920		Crippen Method
mcvol	296.300	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	805.27	K	Joback Method
tc	997.08	K	Joback Method
tf	447.24	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.47	J/molxK	805.27	Joback Method
cpg	934.59	J/molxK	837.24	Joback Method
cpg	951.60	J/molxK	869.21	Joback Method
cpg	967.53	J/molxK	901.17	Joback Method
cpg	982.40	J/molxK	933.14	Joback Method
cpg	996.25	J/molxK	965.11	Joback Method
cpg	1009.11	J/molxK	997.08	Joback Method
dvisc	0.0008017	Paxs	447.24	Joback Method

dvisc	0.0003825	Paxs	506.91	Joback Method
dvisc	0.0002133	Paxs	566.58	Joback Method
dvisc	0.0001329	Paxs	626.25	Joback Method
dvisc	0.0000899	Paxs	685.93	Joback Method
dvisc	0.0000648	Paxs	745.60	Joback Method
dvisc	0.0000490	Paxs	805.27	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=R540886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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