

Sebacic acid, 2-phenoxyethyl propyl ester

Inchi:	InChI=1S/C21H32O5/c1-2-16-25-20(22)14-10-5-3-4-6-11-15-21(23)26-18-17-24-19-12-8
InchiKey:	KWOCQBIVNGOJO-UHFFFAOYSA-N
Formula:	C21H32O5
SMILES:	CCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	364.48

Physical Properties

Property code	Value	Unit	Source
gf	-334.49	kJ/mol	Joback Method
hf	-862.06	kJ/mol	Joback Method
hfus	50.95	kJ/mol	Joback Method
hvap	85.34	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.683		Crippen Method
mvol	303.740	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
rinpol	2687.00		NIST Webbook
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tb	881.56	K	Joback Method
tc	1084.04	K	Joback Method
tf	519.40	K	Joback Method
vc	1.169	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.40	J/molxK	881.56	Joback Method
cpg	1034.55	J/molxK	1050.29	Joback Method
cpg	1023.57	J/molxK	1016.55	Joback Method
cpg	1011.39	J/molxK	982.80	Joback Method
cpg	997.98	J/molxK	949.05	Joback Method
cpg	983.32	J/molxK	915.31	Joback Method
cpg	1044.34	J/molxK	1084.04	Joback Method
dvisc	0.0000350	Paxs	881.56	Joback Method

dvisc	0.0000457	Paxs	821.20	Joback Method
dvisc	0.0000621	Paxs	760.84	Joback Method
dvisc	0.0000890	Paxs	700.48	Joback Method
dvisc	0.0001365	Paxs	640.12	Joback Method
dvisc	0.0002290	Paxs	579.76	Joback Method
dvisc	0.0004332	Paxs	519.40	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=U380780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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