

Sebacic acid, nonyl 2-phenoxyethyl ester

Inchi:	InChI=1S/C27H44O5/c1-2-3-4-5-8-11-17-22-31-26(28)20-15-9-6-7-10-16-21-27(29)32-24
InchiKey:	O UWORABDNVTAQL-UHFFFAOYSA-N
Formula:	C27H44O5
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	448.64

Physical Properties

Property code	Value	Unit	Source
gf	-283.97	kJ/mol	Joback Method
hf	-985.90	kJ/mol	Joback Method
hfus	66.49	kJ/mol	Joback Method
hvap	98.69	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	7.023		Crippen Method
mvol	388.280	ml/mol	McGowan Method
pc	863.02	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	1018.84	K	Joback Method
tc	1251.73	K	Joback Method
tf	587.02	K	Joback Method
vc	1.506	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1336.34	J/molxK	1018.84	Joback Method
cpg	1353.55	J/molxK	1057.66	Joback Method
cpg	1368.89	J/molxK	1096.47	Joback Method
cpg	1382.42	J/molxK	1135.29	Joback Method
cpg	1394.18	J/molxK	1174.10	Joback Method
cpg	1404.24	J/molxK	1212.92	Joback Method
cpg	1412.65	J/molxK	1251.73	Joback Method
dvisc	0.0002090	Paxs	587.02	Joback Method

dvisc	0.0001041	Paxs	658.99	Joback Method
dvisc	0.0000595	Paxs	730.96	Joback Method
dvisc	0.0000376	Paxs	802.93	Joback Method
dvisc	0.0000256	Paxs	874.90	Joback Method
dvisc	0.0000185	Paxs	946.87	Joback Method
dvisc	0.0000140	Paxs	1018.84	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=U380787&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

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