

Fumaric acid, nonyl 4-phenoxybenzyl ester

Inchi:	InChI=1S/C26H32O5/c1-2-3-4-5-6-7-11-20-29-25(27)18-19-26(28)30-21-22-14-16-24(17)
InchiKey:	KHXYWVOKDLKFLD-VHEBQXMUSA-N
Formula:	C26H32O5
SMILES:	CCCCCCCCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	424.53

Physical Properties

Property code	Value	Unit	Source
gf	-109.39	kJ/mol	Joback Method
hf	-622.98	kJ/mol	Joback Method
hfus	57.75	kJ/mol	Joback Method
hvap	99.36	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.372		Crippen Method
mcvol	346.130	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinsol	3228.00		NIST Webbook
tb	1031.78	K	Joback Method
tc	1264.53	K	Joback Method
tf	609.61	K	Joback Method
vc	1.321	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1135.74	J/molxK	1031.78	Joback Method
cpg	1149.20	J/molxK	1070.57	Joback Method
cpg	1161.18	J/molxK	1109.36	Joback Method
cpg	1171.74	J/molxK	1148.15	Joback Method
cpg	1180.96	J/molxK	1186.94	Joback Method
cpg	1188.90	J/molxK	1225.74	Joback Method
cpg	1195.63	J/molxK	1264.53	Joback Method
dvisc	0.0001726	Paxs	609.61	Joback Method
dvisc	0.0000935	Paxs	679.97	Joback Method

dvisc	0.0000569	Paxs	750.33	Joback Method
dvisc	0.0000376	Paxs	820.69	Joback Method
dvisc	0.0000266	Paxs	891.06	Joback Method
dvisc	0.0000198	Paxs	961.42	Joback Method
dvisc	0.0000153	Paxs	1031.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348118&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

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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