Fumaric acid, 4-phenoxybenzyl pentyl ester

Inchi: InChI=1S/C22H24O5/c1-2-3-7-16-25-21(23)14-15-22(24)26-17-18-10-12-20(13-11-18)27
InchiKey: QQVSOLFHKZZSRK-CCEZHUSRSA-N
Formula: C22H24O5
SMILES: CCCCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 368.42

Physical Properties

Property code	Value	Unit	Source
gf	-143.07	kJ/mol	Joback Method
hf	-540.42	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	90.46	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.812		Crippen Method
mcvol	289.770	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	2817.00		NIST Webbook
tb	940.26	K	Joback Method
tc	1166.89	K	Joback Method
tf	564.53	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.88	J/mol×K	940.26	Joback Method
cpg	950.20	J/mol×K	1129.12	Joback Method
cpg	942.01	J/mol×K	1091.35	Joback Method
cpg	932.63	J/mol×K	1053.58	Joback Method
cpg	922.02	J/mol×K	1015.80	Joback Method
cpg	910.11	J/mol×K	978.03	Joback Method
cpg	957.24	J/mol×K	1166.89	Joback Method
dvisc	0.0000277	Pa×s	940.26	Joback Method
dvisc	0.0000354	Pa×s	877.64	Joback Method

dvisc	0.0000470	Pa×s	815.02	Joback Method
dvisc	0.0000654	Pa×s	752.39	Joback Method
dvisc	0.0000966	Pa×s	689.77	Joback Method
dvisc	0.0001543	Pa×s	627.15	Joback Method
dvisc	0.0002733	Pa×s	564.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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