Fumaric acid, 4-phenoxybenzyl propyl ester

Inchi: InChI=1S/C20H20O5/c1-2-14-23-19(21)12-13-20(22)24-15-16-8-10-18(11-9-16)25-17-6-
InchiKey: IECBZSDCEITCPF-OUKQBFOZSA-N
Formula: C20H20O5
SMILES: CCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 340.37

Physical Properties

Property code	Value	Unit	Source
gf	-159.91	kJ/mol	Joback Method
hf	-499.14	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	86.01	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.031		Crippen Method
mcvol	261.590	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	2606.00		NIST Webbook
tb	894.50	K	Joback Method
tc	1123.16	K	Joback Method
tf	541.99	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.88	J/mol×K	894.50	Joback Method
cpg	833.88	J/mol×K	1085.05	Joback Method
cpg	825.70	J/mol×K	1046.94	Joback Method
cpg	816.35	J/mol×K	1008.83	Joback Method
cpg	805.79	J/mol×K	970.72	Joback Method
cpg	793.98	J/mol×K	932.61	Joback Method
cpg	840.93	J/mol×K	1123.16	Joback Method
dvisc	0.0000368	Pa×s	894.50	Joback Method
dvisc	0.0000468	Pa×s	835.75	Joback Method

dvisc	0.0000616	Pa×s	777.00	Joback Method
dvisc	0.0000849	Pa×s	718.25	Joback Method
dvisc	0.0001239	Pa×s	659.49	Joback Method
dvisc	0.0001946	Pa×s	600.74	Joback Method
dvisc	0.0003370	Pa×s	541.99	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=U348110&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