Fumaric acid, octyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C25H30O5/c1-2-3-4-5-6-10-19-28-24(26)17-18-25(27)29-20-21-13-15-23(16-1
InchiKey: SQCQJMONXDFJHZ-ISLYRVAYSA-N
Formula: C25H30O5
SMILES: CCCCCCCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 410.50

Physical Properties

Property code	Value	Unit	Source
gf	-117.81	kJ/mol	Joback Method
hf	-602.34	kJ/mol	Joback Method
hfus	55.16	kJ/mol	Joback Method
hvap	97.14	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.982		Crippen Method
mcvol	332.040	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
rinpol	3125.00		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	1008.90	K	Joback Method
tc	1238.71	K	Joback Method
tf	598.34	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.29	J/mol×K	1008.90	Joback Method
cpg	1128.54	J/mol×K	1200.41	Joback Method
cpg	1120.51	J/mol×K	1162.11	Joback Method
cpg	1111.24	J/mol×K	1123.81	Joback Method
cpg	1100.65	J/mol×K	1085.50	Joback Method
cpg	1088.68	J/mol×K	1047.20	Joback Method
cpg	1135.37	J/mol×K	1238.71	Joback Method
dvisc	0.0000178	Pa×s	1008.90	Joback Method

dvisc	0.0000229	Pa×s	940.47	Joback Method
dvisc	0.0000308	Pa×s	872.05	Joback Method
dvisc	0.0000434	Pa×s	803.62	Joback Method
dvisc	0.0000652	Pa×s	735.19	Joback Method
dvisc	0.0001064	Pa×s	666.77	Joback Method
dvisc	0.0001945	Pa×s	598.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348117&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