Fumaric acid, pentyl 4-phenylphenyl ester

Inchi: InChI=1S/C21H22O4/c1-2-3-7-16-24-20(22)14-15-21(23)25-19-12-10-18(11-13-19)17-8-
InchiKey: JOXTZHCATSAEFL-CCEZHUSRSA-N
Formula: C21H22O4
SMILES: CCCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-46.49	kJ/mol	Joback Method
hf	-387.56	kJ/mol	Joback Method
hfus	43.61	kJ/mol	Joback Method
hvap	85.82	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.549		Crippen Method
mcvol	269.810	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2830.00		NIST Webbook
tb	894.96	K	Joback Method
tc	1122.90	K	Joback Method
tf	531.03	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.56	J/mol×K	894.96	Joback Method
cpg	825.47	J/mol×K	932.95	Joback Method
cpg	838.17	J/mol×K	970.94	Joback Method
cpg	849.72	J/mol×K	1008.93	Joback Method
cpg	860.16	J/mol×K	1046.92	Joback Method
cpg	869.57	J/mol×K	1084.91	Joback Method
cpg	878.01	J/mol×K	1122.90	Joback Method
dvisc	0.0004304	Pa×s	531.03	Joback Method
dvisc	0.0002404	Pa×s	591.68	Joback Method

dvisc	0.0001497	Pa×s	652.34	Joback Method
dvisc	0.0001010	Pa×s	713.00	Joback Method
dvisc	0.0000725	Pa×s	773.65	Joback Method
dvisc	0.0000546	Pa×s	834.31	Joback Method
dvisc	0.0000427	Pa×s	894.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348210&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