Fumaric acid, butyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C21H22O5/c1-2-3-15-24-20(22)13-14-21(23)25-16-17-9-11-19(12-10-17)26-18
InchiKey: LFSGXOWDOWBBFO-BUHFOSPRSA-N
Formula: C21H22O5
SMILES: CCCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 354.40

Physical Properties

Property code	Value	Unit	Source
gf	-151.49	kJ/mol	Joback Method
hf	-519.78	kJ/mol	Joback Method
hfus	44.80	kJ/mol	Joback Method
hvap	88.23	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.422		Crippen Method
mcvol	275.680	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2713.00		NIST Webbook
rinpol	2713.00		NIST Webbook
tb	917.38	K	Joback Method
tc	1144.64	K	Joback Method
tf	553.26	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.55	J/mol×K	917.38	Joback Method
cpg	851.72	J/mol×K	955.26	Joback Method
cpg	863.59	J/mol×K	993.13	Joback Method
cpg	874.19	J/mol×K	1031.01	Joback Method
cpg	883.57	J/mol×K	1068.89	Joback Method
cpg	891.77	J/mol×K	1106.77	Joback Method
cpg	898.83	J/mol×K	1144.64	Joback Method
dvisc	0.0003041	Pa×s	553.26	Joback Method

dvisc	0.0001736	Pa×s	613.95	Joback Method
dvisc	0.0001096	Pa×s	674.63	Joback Method
dvisc	0.0000747	Pa×s	735.32	Joback Method
dvisc	0.0000539	Pa×s	796.01	Joback Method
dvisc	0.0000408	Pa×s	856.69	Joback Method
dvisc	0.0000320	Pa×s	917.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348112&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