

Fumaric acid, isobutyl 4-phenoxybenzyl ester

Inchi:	InChI=1S/C21H22O5/c1-16(2)14-24-20(22)12-13-21(23)25-15-17-8-10-19(11-9-17)26-18
InchiKey:	TWLMOCDQUHXQDK-OUKQBFOZSA-N
Formula:	C21H22O5
SMILES:	CC(C)COC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	354.40

Physical Properties

Property code	Value	Unit	Source
gf	-153.93	kJ/mol	Joback Method
hf	-525.06	kJ/mol	Joback Method
hfus	41.28	kJ/mol	Joback Method
hvap	87.85	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.277		Crippen Method
mcvol	275.680	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2662.00		NIST Webbook
tb	916.94	K	Joback Method
tc	1146.76	K	Joback Method
tf	538.26	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.06	J/molxK	916.94	Joback Method
cpg	852.34	J/molxK	955.24	Joback Method
cpg	864.26	J/molxK	993.55	Joback Method
cpg	874.88	J/molxK	1031.85	Joback Method
cpg	884.24	J/molxK	1070.15	Joback Method
cpg	892.37	J/molxK	1108.46	Joback Method
cpg	899.33	J/molxK	1146.76	Joback Method
dvisc	0.0003342	Paxs	538.26	Joback Method
dvisc	0.0001799	Paxs	601.37	Joback Method

dvisc	0.0001089	Paxs	664.49	Joback Method
dvisc	0.0000720	Paxs	727.60	Joback Method
dvisc	0.0000508	Paxs	790.71	Joback Method
dvisc	0.0000377	Paxs	853.83	Joback Method
dvisc	0.0000292	Paxs	916.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348111&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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