Fumaric acid, 4-chlorobenzyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C17H21ClO4/c1-4-15(12(2)3)22-17(20)10-9-16(19)21-11-13-5-7-14(18)8-6-13/

InchiKey: HJRGLLKANKNFMH-MDZDMXLPSA-N

Formula: C17H21ClO4

SMILES: CCC(OC(=O)C=CC(=O)OCc1ccc(Cl)cc1)C(C)C

Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-209.39	kJ/mol	Joback Method
hf	-567.83	kJ/mol	Joback Method
hfus	36.37	kJ/mol	Joback Method
hvap	78.25	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.917		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	813.31	K	Joback Method
tc	1028.90	K	Joback Method
tf	459.45	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.40	J/mol×K	813.31	Joback Method
cpg	720.54	J/mol×K	849.24	Joback Method
cpg	733.60	J/mol×K	885.17	Joback Method
cpg	745.64	J/mol×K	921.11	Joback Method
cpg	756.68	J/mol×K	957.04	Joback Method
cpg	766.75	J/mol×K	992.97	Joback Method
cpg	775.89	J/mol×K	1028.90	Joback Method
dvisc	0.0007896	Pa×s	459.45	Joback Method

dvisc	0.0003896	Pa×s	518.43	Joback Method
dvisc	0.0002221	Pa×s	577.40	Joback Method
dvisc	0.0001405	Pa×s	636.38	Joback Method
dvisc	0.0000960	Pa×s	695.36	Joback Method
dvisc	0.0000697	Pa×s	754.33	Joback Method
dvisc	0.0000530	Pa×s	813.31	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=U405915&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