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

Inchi: InChI=1S/C16H19ClO4/c1-11(2)12(3)21-16(19)9-8-15(18)20-10-13-4-6-14(17)7-5-13/h4-

InchiKey: AMEIIMGIDHGYFG-CMDGGOBGSA-N

Formula: C16H19ClO4

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

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-217.81	kJ/mol	Joback Method
hf	-547.19	kJ/mol	Joback Method
hfus	33.77	kJ/mol	Joback Method
hvap	76.03	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.527		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	790.43	K	Joback Method
tc	1008.24	K	Joback Method
tf	448.18	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.77	J/mol×K	790.43	Joback Method
cpg	710.01	J/mol×K	971.94	Joback Method
cpg	700.12	J/mol×K	935.63	Joback Method
cpg	689.28	J/mol×K	899.33	Joback Method
cpg	677.46	J/mol×K	863.03	Joback Method
cpg	664.64	J/mol×K	826.73	Joback Method
cpg	718.98	J/mol×K	1008.24	Joback Method
dvisc	0.0000608	Pa×s	790.43	Joback Method

dvisc	0.0000797	Pa×s	733.39	Joback Method
dvisc	0.0001095	Pa×s	676.35	Joback Method
dvisc	0.0001594	Pa×s	619.31	Joback Method
dvisc	0.0002505	Pa×s	562.26	Joback Method
dvisc	0.0004359	Pa×s	505.22	Joback Method
dvisc	0.0008734	Pa×s	448.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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