

Fumaric acid, butyl 2-chloro-5-methylphenyl ester

Inchi:	InChI=1S/C15H17ClO4/c1-3-4-9-19-14(17)7-8-15(18)20-13-10-11(2)5-6-12(13)16/h5-8,1
InchiKey:	FNERJLZUNQETKU-BQYQJAHWSA-N
Formula:	C15H17ClO4
SMILES:	CCCCOC(=O)C=CC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	296.75

Physical Properties

Property code	Value	Unit	Source
gf	-230.98	kJ/mol	Joback Method
hf	-527.46	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.453		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinsol	2140.00		NIST Webbook
tb	773.41	K	Joback Method
tc	987.91	K	Joback Method
tf	479.43	K	Joback Method
vc	0.845	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.74	J/molxK	773.41	Joback Method
cpg	606.78	J/molxK	809.16	Joback Method
cpg	618.90	J/molxK	844.91	Joback Method
cpg	630.12	J/molxK	880.66	Joback Method
cpg	640.46	J/molxK	916.41	Joback Method
cpg	649.94	J/molxK	952.16	Joback Method
cpg	658.58	J/molxK	987.91	Joback Method
dvisc	0.0006170	Paxs	479.43	Joback Method
dvisc	0.0003777	Paxs	528.43	Joback Method

dvisc	0.0002513	Paxs	577.42	Joback Method
dvisc	0.0001782	Paxs	626.42	Joback Method
dvisc	0.0001328	Paxs	675.42	Joback Method
dvisc	0.0001030	Paxs	724.41	Joback Method
dvisc	0.0000825	Paxs	773.41	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=U348257&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

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