

Fumaric acid, 2-chlorophenyl hept-2-yl ester

Inchi: InChI=1S/C17H21ClO4/c1-3-4-5-8-13(2)21-16(19)11-12-17(20)22-15-10-7-6-9-14(15)18/
InchiKey: RXZCFPFPHIKPNN-VAWYXSNFSA-N
Formula: C17H21ClO4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-206.95	kJ/mol	Joback Method
hf	-562.55	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	78.64	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.314		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpola	2229.00		NIST Webbook
rinpola	2229.00		NIST Webbook
tb	813.75	K	Joback Method
tc	1026.45	K	Joback Method
tf	474.45	K	Joback Method
vc	0.951	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.84	J/molxK	813.75	Joback Method
cpg	719.79	J/molxK	849.20	Joback Method
cpg	732.71	J/molxK	884.65	Joback Method
cpg	744.65	J/molxK	920.10	Joback Method
cpg	755.62	J/molxK	955.55	Joback Method
cpg	765.67	J/molxK	991.00	Joback Method
cpg	774.82	J/molxK	1026.45	Joback Method
dvisc	0.0006850	Paxs	474.45	Joback Method

dvisc	0.0003641	Paxs	531.00	Joback Method
dvisc	0.0002186	Paxs	587.55	Joback Method
dvisc	0.0001435	Paxs	644.10	Joback Method
dvisc	0.0001009	Paxs	700.65	Joback Method
dvisc	0.0000747	Paxs	757.20	Joback Method
dvisc	0.0000577	Paxs	813.75	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=U405723&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

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