Fumaric acid, 4-chlorobenzyl hept-2-yl ester

Inchi: InChI=1S/C18H23ClO4/c1-3-4-5-6-14(2)23-18(21)12-11-17(20)22-13-15-7-9-16(19)10-8-
InchiKey: CUMZQXHDJYYOMQ-VAWYXSNFSA-N
Formula: C18H23ClO4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]: 338.83

Physical Properties

Property code	Value	Unit	Source
gf	-198.53	kJ/mol	Joback Method
hf	-583.19	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.451		Crippen Method
mcvol	263.540	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2394.00		NIST Webbook
rinpol	2394.00		NIST Webbook
tb	836.63	K	Joback Method
tc	1048.04	K	Joback Method
tf	485.72	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.42	J/mol×K	836.63	Joback Method
cpg	823.27	J/mol×K	1012.80	Joback Method
cpg	813.06	J/mol×K	977.57	Joback Method
cpg	801.91	J/mol×K	942.33	Joback Method
cpg	789.77	J/mol×K	907.10	Joback Method
cpg	776.62	J/mol×K	871.86	Joback Method
cpg	832.56	J/mol×K	1048.04	Joback Method
dvisc	0.0000502	Pa×s	836.63	Joback Method

dvisc	0.0000652	Pa×s	778.14	Joback Method
dvisc	0.0000884	Pa×s	719.66	Joback Method
dvisc	0.0001264	Pa×s	661.17	Joback Method
dvisc	0.0001937	Pa×s	602.69	Joback Method
dvisc	0.0003254	Pa×s	544.21	Joback Method
dvisc	0.0006195	Pa×s	485.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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