Fumaric acid, 4-chlorobenzyl cyclohexylmethyl ester

Inchi: InChI=1S/C18H21ClO4/c19-16-8-6-15(7-9-16)13-23-18(21)11-10-17(20)22-12-14-4-2-1-3

InchiKey: OUFFLBQIOSCALW-ZHACJKMWSA-N

Formula: C18H21ClO4

SMILES: O=C(C=CC(=O)OCC1CCCCC1)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 336.81

Physical Properties

Property code	Value	Unit	Source
gf	-171.64	kJ/mol	Joback Method
hf	-523.59	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	81.68	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.063		Crippen Method
mcvol	252.680	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	856.62	K	Joback Method
tc	1089.69	K	Joback Method
tf	508.10	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.45	J/mol×K	856.62	Joback Method
cpg	817.22	J/mol×K	1050.85	Joback Method
cpg	807.47	J/mol×K	1012.00	Joback Method
cpg	796.46	J/mol×K	973.16	Joback Method
cpg	784.16	J/mol×K	934.31	Joback Method
cpg	770.50	J/mol×K	895.47	Joback Method
cpg	825.77	J/mol×K	1089.69	Joback Method
dvisc	0.0000568	Pa×s	856.62	Joback Method

dvisc	0.0000732	Pa×s	798.53	Joback Method
dvisc	0.0000983	Pa×s	740.45	Joback Method
dvisc	0.0001387	Pa×s	682.36	Joback Method
dvisc	0.0002087	Pa×s	624.27	Joback Method
dvisc	0.0003415	Pa×s	566.19	Joback Method
dvisc	0.0006253	Pa×s	508.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405920&Units=SI

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