Fumaric acid, 4-chlorobenzyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C16H17ClO4/c1-12(2)9-10-20-15(18)7-8-16(19)21-11-13-3-5-14(17)6-4-13/h3-

InchiKey: PEKUSRMEMWLCTM-BQYQJAHWSA-N

Formula: C16H17ClO4

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

Mol. weight [g/mol]: 308.76

Physical Properties

Property code	Value	Unit	Source
gf	-141.26	kJ/mol	Joback Method
hf	-429.20	kJ/mol	Joback Method
hfus	39.71	kJ/mol	Joback Method
hvap	76.84	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.449		Crippen Method
mcvol	231.060	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
tb	795.35	K	Joback Method
tc	1016.12	K	Joback Method
tf	459.14	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.46	J/mol×K	795.35	Joback Method
cpg	636.57	J/mol×K	832.15	Joback Method
cpg	648.73	J/mol×K	868.94	Joback Method
cpg	659.99	J/mol×K	905.74	Joback Method
cpg	670.41	J/mol×K	942.53	Joback Method
cpg	680.02	J/mol×K	979.33	Joback Method
cpg	688.89	J/mol×K	1016.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405916&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

Legend

cpg:	Ideal gas heat capacity
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