

Fumaric acid, 4-octyl 1,1,1-trifluoroprop-2-yl ester

Inchi:	InChI=1S/C15H23F3O4/c1-4-6-8-12(7-5-2)22-14(20)10-9-13(19)21-11(3)15(16,17)18/h9
InchiKey:	JJMHRXAGGIKJLF-MDZDMXLPSA-N
Formula:	C15H23F3O4
SMILES:	CCCCC(CCC)OC(=O)C=CC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]:	324.34

Physical Properties

Property code	Value	Unit	Source
gf	-898.67	kJ/mol	Joback Method
hf	-1332.95	kJ/mol	Joback Method
hfus	35.16	kJ/mol	Joback Method
hvap	62.73	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.939		Crippen Method
mcvol	238.100	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	693.04	K	Joback Method
tc	868.58	K	Joback Method
tf	372.24	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.61	J/mol×K	693.04	Joback Method
cpg	696.46	J/mol×K	722.30	Joback Method
cpg	710.51	J/mol×K	751.55	Joback Method
cpg	723.79	J/mol×K	780.81	Joback Method
cpg	736.32	J/mol×K	810.07	Joback Method
cpg	748.14	J/mol×K	839.32	Joback Method
cpg	759.26	J/mol×K	868.58	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=U405618&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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