Fumaric acid, pentafluorobenzyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C16H13F5O4/c1-8(2)5-6-24-10(22)3-4-11(23)25-7-9-12(17)14(19)16(21)15(20

InchiKey: PNHTVLINRZLSPW-ONEGZZNKSA-N

Formula: C16H13F5O4

SMILES: CC(C)=CCOC(=O)C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 364.26

Physical Properties

Property code	Value	Unit	Source
gf	-1141.90	kJ/mol	Joback Method
hf	-1439.89	kJ/mol	Joback Method
hfus	49.36	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.491		Crippen Method
mcvol	227.670	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	774.19	K	Joback Method
tc	963.48	K	Joback Method
tf	482.25	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.81	J/mol×K	774.19	Joback Method
cpg	644.26	J/mol×K	805.74	Joback Method
cpg	655.01	J/mol×K	837.29	Joback Method
cpg	665.09	J/mol×K	868.83	Joback Method
cpg	674.50	J/mol×K	900.38	Joback Method
cpg	683.26	J/mol×K	931.93	Joback Method
cpg	691.38	J/mol×K	963.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405878&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
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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