Fumaric acid, monoamide, N-allyl-, pentafluorobenzyl ester

Inchi: InChI=1S/C14H10F5NO3/c1-2-5-20-8(21)3-4-9(22)23-6-7-10(15)12(17)14(19)13(18)11(7

InchiKey: RBYLQSLCYFPNTO-ONEGZZNKSA-N

Formula: C14H10F5NO3

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

Mol. weight [g/mol]: 335.23

Physical Properties

Property code	Value	Unit	Source
gf	-948.18	kJ/mol	Joback Method
hf	-1194.92	kJ/mol	Joback Method
hfus	47.92	kJ/mol	Joback Method
hvap	69.89	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	2.284		Crippen Method
mcvol	203.600	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	2107.00		NIST Webbook
tb	748.82	K	Joback Method
tc	936.47	K	Joback Method
tf	507.42	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.30	J/mol×K	748.82	Joback Method
cpg	562.51	J/mol×K	780.10	Joback Method
cpg	572.10	J/mol×K	811.37	Joback Method
cpg	581.08	J/mol×K	842.65	Joback Method
cpg	589.46	J/mol×K	873.92	Joback Method
cpg	597.26	J/mol×K	905.20	Joback Method
cpg	604.51	J/mol×K	936.47	Joback Method

Sources

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=U357448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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