Fumaric acid, 2-pentyl 2-fluorophenyl ester

Inchi: InChI=1S/C15H17FO4/c1-3-6-11(2)19-14(17)9-10-15(18)20-13-8-5-4-7-12(13)16/h4-5,7-
InchiKey: WEKBUCGGTOVYJT-MDZDMXLPSA-N
Formula: C15H17FO4
SMILES: CCCC(C)OC(=O)C=CC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 280.29

Physical Properties

Property code	Value	Unit	Source
gf	-406.67	kJ/mol	Joback Method
hf	-701.64	kJ/mol	Joback Method
hfus	33.59	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.019		Crippen Method
mcvol	210.800	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1861.00		NIST Webbook
rinpol	1861.00		NIST Webbook
tb	729.83	K	Joback Method
tc	935.84	K	Joback Method
tf	422.58	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.05	J/mol×K	729.83	Joback Method
cpg	591.92	J/mol×K	764.17	Joback Method
cpg	604.88	J/mol×K	798.50	Joback Method
cpg	616.95	J/mol×K	832.84	Joback Method
cpg	628.15	J/mol×K	867.17	Joback Method
cpg	638.50	J/mol×K	901.51	Joback Method
cpg	648.02	J/mol×K	935.84	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=U405560&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/93-550-8/Fumaric-acid-2-pentyl-2-fluorophenyl-ester.pdf
Generated by Cheméo on 2024-04-28 19:54:22.614769249 +0000 UTC m=+16623311.535346571.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.