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

Inchi: InChI=1S/C15H23F3O4/c1-10(8-14(3,4)5)9-21-12(19)6-7-13(20)22-11(2)15(16,17)18/h6-

InchiKey: SELFXULHXLTZEO-VOTSOKGWSA-N

Formula: C15H23F3O4

SMILES: CC(COC(=O)C=CC(=O)OC(C)C(F)(F)F)CC(C)(C)C

Mol. weight [g/mol]: 324.34

Physical Properties

Property code	Value	Unit	Source
gf	-895.83	kJ/mol	Joback Method
hf	-1341.70	kJ/mol	Joback Method
hfus	27.75	kJ/mol	Joback Method
hvap	61.44	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.652		Crippen Method
mcvol	238.100	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
tb	689.81	K	Joback Method
tc	871.60	K	Joback Method
tf	374.66	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.11	J/mol×K	689.81	Joback Method
cpg	699.28	J/mol×K	720.11	Joback Method
cpg	713.57	J/mol×K	750.41	Joback Method
cpg	727.01	J/mol×K	780.70	Joback Method
cpg	739.65	J/mol×K	811.00	Joback Method
cpg	751.52	J/mol×K	841.30	Joback Method
cpg	762.68	J/mol×K	871.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405597&Units=SI

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