Succinic acid, 3-fluorobenzyl heptyl ester

Inchi: InChI=1S/C18H25FO4/c1-2-3-4-5-6-12-22-17(20)10-11-18(21)23-14-15-8-7-9-16(19)13-1
InchiKey: LQIRSNFNWHXTDN-UHFFFAOYSA-N
Formula: C18H25FO4
SMILES: CCCCCCCOC(=O)CCC(=O)OCc1cccc(F)c1
Mol. weight [g/mol]: 324.39

Physical Properties

Property code	Value	Unit	Source
gf	-459.19	kJ/mol	Joback Method
hf	-875.50	kJ/mol	Joback Method
hfus	44.68	kJ/mol	Joback Method
hvap	76.09	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.163		Crippen Method
mcvol	257.370	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	794.75	K	Joback Method
tc	989.35	K	Joback Method
tf	476.47	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.80	J/mol×K	794.75	Joback Method
cpg	783.99	J/mol×K	827.18	Joback Method
cpg	798.18	J/mol×K	859.62	Joback Method
cpg	811.39	J/mol×K	892.05	Joback Method
cpg	823.64	J/mol×K	924.48	Joback Method
cpg	834.94	J/mol×K	956.92	Joback Method
cpg	845.31	J/mol×K	989.35	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=U381241&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

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