

Succinic acid, 4-fluorobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H25FO4/c1-4-5-16(13(2)3)23-18(21)11-10-17(20)22-12-14-6-8-15(19)9-7-
InchiKey:	XRWKWVLGFPBEAD-UHFFFAOYSA-N
Formula:	C18H25FO4
SMILES:	CCCC(OC(=O)CCC(=O)OCc1ccc(F)cc1)C(C)C
Mol. weight [g/mol]:	324.39

Physical Properties

Property code	Value	Unit	Source
gf	-464.07	kJ/mol	Joback Method
hf	-886.06	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	75.32	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.017		Crippen Method
mvol	257.370	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	793.87	K	Joback Method
tc	992.71	K	Joback Method
tf	446.47	K	Joback Method
vc	0.990	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.87	J/mol×K	793.87	Joback Method
cpg	785.39	J/mol×K	827.01	Joback Method
cpg	799.85	J/mol×K	860.15	Joback Method
cpg	813.27	J/mol×K	893.29	Joback Method
cpg	825.66	J/mol×K	926.43	Joback Method
cpg	837.04	J/mol×K	959.57	Joback Method
cpg	847.43	J/mol×K	992.71	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=U381672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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