

Sebacic acid, 2-fluorophenyl heptyl ester

Inchi:	InChI=1S/C23H35FO4/c1-2-3-4-9-14-19-27-22(25)17-10-7-5-6-8-11-18-23(26)28-21-16-
InchiKey:	KBVSVKLLDMXAIA-UHFFFAOYSA-N
Formula:	C23H35FO4
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)Oc1ccccc1F
Mol. weight [g/mol]:	394.52

Physical Properties

Property code	Value	Unit	Source
gf	-417.09	kJ/mol	Joback Method
hf	-978.70	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	87.22	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.365		Crippen Method
mvol	327.820	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	2802.00		NIST Webbook
rinpol	2802.00		NIST Webbook
tb	909.15	K	Joback Method
tc	1113.70	K	Joback Method
tf	532.82	K	Joback Method
vc	1.282	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.16	J/molxK	909.15	Joback Method
cpg	1081.71	J/molxK	943.24	Joback Method
cpg	1096.99	J/molxK	977.33	Joback Method
cpg	1111.03	J/molxK	1011.42	Joback Method
cpg	1123.86	J/molxK	1045.51	Joback Method
cpg	1135.51	J/molxK	1079.61	Joback Method
cpg	1146.01	J/molxK	1113.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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