

Sebacic acid, butyl 2,5-difluorobenzyl ester

Inchi: InChI=1S/C21H30F2O4/c1-2-3-14-26-20(24)10-8-6-4-5-7-9-11-21(25)27-16-17-15-18(22)
InchiKey: AVMXKOIZTSM TDR-UHFFFAOYSA-N
Formula: C21H30F2O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 384.46

Physical Properties

Property code	Value	Unit	Source
gf	-638.37	kJ/mol	Joback Method
hf	-1145.00	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.472		Crippen Method
mvol	301.410	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook
tb	867.64	K	Joback Method
tc	1064.57	K	Joback Method
tf	523.39	K	Joback Method
vc	1.188	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.07	J/mol×K	867.64	Joback Method
cpg	966.71	J/mol×K	900.46	Joback Method
cpg	981.22	J/mol×K	933.28	Joback Method
cpg	994.62	J/mol×K	966.10	Joback Method
cpg	1006.93	J/mol×K	998.92	Joback Method
cpg	1018.17	J/mol×K	1031.75	Joback Method
cpg	1028.36	J/mol×K	1064.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U380763&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
hvpap:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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