Succinic acid, tridec-2-yn-1-yl pentafluorobenzyl ester

Inchi: InChI=1S/C24H29F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-32-18(30)13-14-19(31)33-16-17

InchiKey: YTRKQZGMLQSLQJ-UHFFFAOYSA-N

Formula: C24H29F5O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 476.48

Physical Properties

Property code	Value	Unit	Source
gf	-1023.63	kJ/mol	Joback Method
hf	-1557.36	kJ/mol	Joback Method
hfus	74.11	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	6.283		Crippen Method
mcvol	340.390	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	958.03	K	Joback Method
tc	1174.39	K	Joback Method
tf	702.63	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.07	J/mol×K	958.03	Joback Method
cpg	1110.78	J/mol×K	994.09	Joback Method
cpg	1124.07	J/mol×K	1030.15	Joback Method
cpg	1135.96	J/mol×K	1066.21	Joback Method
cpg	1146.47	J/mol×K	1102.27	Joback Method
cpg	1155.60	J/mol×K	1138.33	Joback Method
cpg	1163.38	J/mol×K	1174.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389895&Units=SI
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

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