2,5-Di(trifluoromethyl)benzoic acid, pentafluorobenzyl ester

Inchi: InChI=1S/C16H5F11O2/c17-9-7(10(18)12(20)13(21)11(9)19)4-29-14(28)6-3-5(15(22,23)
InchiKey: YAISAQIUKATIQO-UHFFFAOYSA-N
Formula: C16H5F11O2
SMILES: O=C(OCc1c(F)c(F)c(F)c(F)c1F)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 438.19

Physical Properties

Property code	Value	Unit	Source
gf	-2129.90	kJ/mol	Joback Method
hf	-2400.31	kJ/mol	Joback Method
hfus	44.39	kJ/mol	Joback Method
hvap	57.97	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	5.777		Crippen Method
mcvol	215.690	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	1546.00		NIST Webbook
tb	715.50	K	Joback Method
tc	891.69	K	Joback Method
tf	494.05	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.91	J/mol×K	715.50	Joback Method
cpg	613.82	J/mol×K	744.87	Joback Method
cpg	623.06	J/mol×K	774.23	Joback Method
cpg	631.65	J/mol×K	803.60	Joback Method
cpg	639.62	J/mol×K	832.96	Joback Method
cpg	647.00	J/mol×K	862.33	Joback Method
cpg	653.83	J/mol×K	891.69	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=U357367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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