Benzoic acid, (4-(trifluoromethyl)phenyl)methyl ester

Inchi: InChI=1S/C15H11F3O2/c16-15(17,18)13-8-6-11(7-9-13)10-20-14(19)12-4-2-1-3-5-12/h1-

InchiKey: UMZAUSNEEFIVRJ-UHFFFAOYSA-N

Formula: C15H11F3O2

SMILES: O=C(OCc1ccc(C(F)(F)F)cc1)c1ccccc1

Mol. weight [g/mol]: 280.24

Physical Properties

Property code	Value	Unit	Source
gf	-524.90	kJ/mol	Joback Method
hf	-733.22	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.062		Crippen Method
mcvol	187.440	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
tb	671.81	K	Joback Method
tc	891.88	K	Joback Method
tf	400.52	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.85	J/mol×K	671.81	Joback Method
cpg	506.80	J/mol×K	708.49	Joback Method
cpg	519.63	J/mol×K	745.17	Joback Method
cpg	531.42	J/mol×K	781.84	Joback Method
cpg	542.21	J/mol×K	818.52	Joback Method
cpg	552.08	J/mol×K	855.20	Joback Method
cpg	561.10	J/mol×K	891.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368705&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