1-Heptafluorobutyryloxy-2-phenylethane

Other names: 2-Phenylethanol, heptafluorobutanoate
Inchi: InChI=1S/C12H9F7O2/c13-10(14,11(15,16)12(17,18)19)9(20)21-7-6-8-4-2-1-3-5-8/h1-5H
InchiKey: HUHVUDFNUXMVGY-UHFFFAOYSA-N
Formula: C12H9F7O2
SMILES: O=C(OCCc1ccccc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 318.19
CAS: 81089-49-8

Physical Properties

Property code	Value	Unit	Source
gf	-1426.50	kJ/mol	Joback Method
hf	-1698.30	kJ/mol	Joback Method
hfus	22.98	kJ/mol	Joback Method
hvap	44.13	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.605		Crippen Method
mcvol	176.010	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
tb	562.13	K	Joback Method
tc	738.93	K	Joback Method
tf	334.97	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.15	J/mol×K	562.13	Joback Method
cpg	474.18	J/mol×K	591.60	Joback Method
cpg	486.27	J/mol×K	621.06	Joback Method
cpg	497.47	J/mol×K	650.53	Joback Method
cpg	507.83	J/mol×K	680.00	Joback Method
cpg	517.41	J/mol×K	709.47	Joback Method

cpg	526.27	J/mol×K	738.93	Joback Method

Sources

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=C81089498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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