Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 4-bromophenyl ester

Inchi: InChI=1S/C15H11BrF8O4/c16-8-1-3-9(4-2-8)28-11(26)6-5-10(25)27-7-13(19,20)15(23,24

InchiKey: CSGCYOZGOURNLI-UHFFFAOYSA-N

Formula: C15H11BrF8O4

SMILES: O=C(CCC(=O)Oc1ccc(Br)cc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 487.14

Physical Properties

Property code	Value	Unit	Source
gf	-1827.72	kJ/mol	Joback Method
hf	-2191.55	kJ/mol	Joback Method
hfus	37.99	kJ/mol	Joback Method
hvap	65.86	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.849		Crippen Method
mcvol	244.990	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	2041.00		NIST Webbook
tb	777.03	K	Joback Method
tc	967.29	K	Joback Method
tf	498.85	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.35	J/mol×K	777.03	Joback Method
cpg	710.59	J/mol×K	808.74	Joback Method
cpg	720.01	J/mol×K	840.45	Joback Method
cpg	728.67	J/mol×K	872.16	Joback Method
cpg	736.64	J/mol×K	903.87	Joback Method
cpg	743.99	J/mol×K	935.58	Joback Method
cpg	750.77	J/mol×K	967.29	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=U389818&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