Succinic acid, cyclohexylmethyl 4-bromophenyl ester

Inchi: InChI=1S/C17H21BrO4/c18-14-6-8-15(9-7-14)22-17(20)11-10-16(19)21-12-13-4-2-1-3-5-

InchiKey: DRNAZRMDDNCFTI-UHFFFAOYSA-N

Formula: C17H21BrO4

SMILES: O=C(CCC(=O)Oc1ccc(Br)cc1)OCC1CCCCC1

Mol. weight [g/mol]: 369.25

Physical Properties

Property code	Value	Unit	Source
gf	-234.03	kJ/mol	Joback Method
hf	-578.10	kJ/mol	Joback Method
hfus	36.13	kJ/mol	Joback Method
hvap	81.55	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.258		Crippen Method
mcvol	248.150	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
tb	858.31	K	Joback Method
tc	1093.87	K	Joback Method
tf	531.79	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.39	J/mol×K	858.31	Joback Method
cpg	752.15	J/mol×K	897.57	Joback Method
cpg	765.48	J/mol×K	936.83	Joback Method
cpg	777.40	J/mol×K	976.09	Joback Method
cpg	787.96	J/mol×K	1015.35	Joback Method
cpg	797.19	J/mol×K	1054.61	Joback Method
cpg	805.14	J/mol×K	1093.87	Joback Method
dvisc	0.0006076	Pa×s	531.79	Joback Method

dvisc	0.0003575	Pa×s	586.21	Joback Method
dvisc	0.0002301	Pa×s	640.63	Joback Method
dvisc	0.0001587	Pa×s	695.05	Joback Method
dvisc	0.0001156	Pa×s	749.47	Joback Method
dvisc	0.0000878	Pa×s	803.89	Joback Method
dvisc	0.0000691	Pa×s	858.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389826&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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