Bis(2-ethylhexyl) methylenesuccinate

Other names: Butanedioic acid, 2-methylene, di(2-ethylhexyl) ester
Inchi: InChI=1S/C21H38O4/c1-6-10-12-18(8-3)15-24-20(22)14-17(5)21(23)25-16-19(9-4)13-11
InchiKey: CGNRQCGWXXLTIA-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: C=C(CC(=O)OCC(CC)CCCC)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 354.52
CAS: 2287-83-4

Physical Properties

Property code	Value	Unit	Source
gf	-267.49	kJ/mol	Joback Method
hf	-861.29	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	79.29	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.452		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
tb	828.14	K	Joback Method
tc	1017.35	K	Joback Method
tf	425.03	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.36	J/mol×K	828.14	Joback Method
cpg	1021.68	J/mol×K	859.67	Joback Method
cpg	1038.88	J/mol×K	891.21	Joback Method
cpg	1055.01	J/mol×K	922.74	Joback Method
cpg	1070.07	J/mol×K	954.28	Joback Method
cpg	1084.09	J/mol×K	985.81	Joback Method
cpg	1097.11	J/mol×K	1017.35	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=C2287834&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume